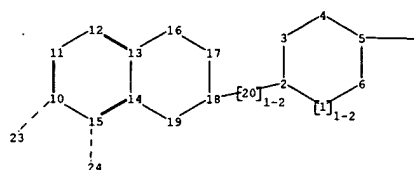
C¹O²N³2¹26²2³

chain nodes :

7 20

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15 16 17 18 19 23 24 25 26 27

chain bonds :

2-20 5-7 18-20

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 10-23 11-12 12-13 13-14 13-16 14-15
14-19 15-24 16-17 17-18 18-19

exact/norm bonds :

1-2 1-6 2-3 2-20 3-4 4-5 5-6 5-7 10-23 13-16 14-19 15-24 16-17 17-18 18-19

exact bonds :

18-20

normalized bonds :

10-11 10-15 11-12 12-13 13-14 14-15

G1:[*1],[*2],[*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 23:Atom 24:Atom
25:Atom 26:Atom 27:Atom

Generic attributes :

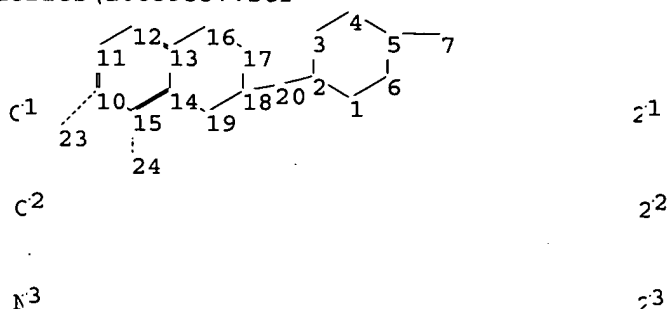
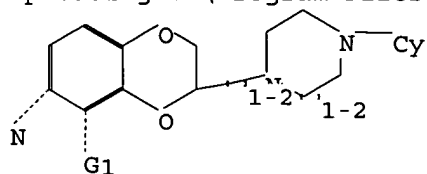
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Saturation : Unsaturated

10/659537

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Uploading C:\Program Files\Stnexp\Queries\10659537.str



chain nodes :

7 20

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15 16 17 18 19 23 24 25 26 27

chain bonds :

2-20 5-7 18-20

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 10-23 11-12 12-13 13-14 13-16

14-15 14-19 15-24 16-17 17-18 18-19

exact/norm bonds :

1-2 1-6 2-3 2-20 3-4 4-5 5-6 5-7 10-23 13-16 14-19 15-24 16-17 17-18

18-19

exact bonds :

18-20

normalized bonds :

10-11 10-15 11-12 12-13 13-14 14-15

G1: [*1], [*2], [*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 10:Atom 11:Atom 12:Atom

13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 23:Atom

24:Atom 25:Atom 26:Atom 27:Atom

Generic attributes :

7:

Saturation : Unsaturated

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 16:32:24 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 7 TO ITERATE

100.0% PROCESSED 7 ITERATIONS

5 ANSWERS

10/659537

.SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 7 TO 298
PROJECTED ANSWERS: 5 TO 234

L2 5 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 16:32:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 89 TO ITERATE

100.0% PROCESSED 89 ITERATIONS 54 ANSWERS
SEARCH TIME: 00.00.01

L3 54 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

	SINCE FILE ENTRY	TOTAL SESSION
	161.33	161.75

FILE 'CAPLUS' ENTERED AT 16:32:36 ON 07 FEB 2005
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FILE COVERS 1907 - 7 Feb 2005 VOL 142 ISS 7
FILE LAST UPDATED: 6 Feb 2005 (20050206/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

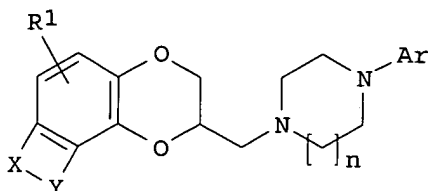
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10/659537

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:589245 CAPLUS
DN 141:123658
TI Preparation of antidepressant arylpiperazine derivatives of
heterocycle-fused benzodioxans
IN Evrard, Deborah Ann; Zhou, Dahui; Stack, Gary Paul; Venkatesan, Aranapakam
Madumbai; Failli, Amedeo A.; Croce, Susan Christman
PA USA
SO U.S. Pat. Appl. Publ., 30 pp., Cont.-in-part of U.S. Provisional Ser. No.
410,082.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

App's

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004142926	A1	20040722	US 2003-659537	20030910
	WO 2004024731	A1	20040325	WO 2003-US28453	20030911
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
PRAI	US 2002-410082P	P	20020912		
	US 2003-659537	A	20030910		
OS	MARPAT 141:123658				
GI					



I

AB The title compds. [I; R1 = H, halo, CN, carboxamido, etc.; XY = N:CR2CR3:N, N:CR2CR4:CH, N:CR2N:CH, N:CR2O, NHCR5:CH; R2, R3 = H, halo, NH2, mono- or dialkylamino, alkyl; R4 = H, alkyl; R5 = H, halo, CF3, pentafluoroethyl, alkyl; Ar = (un)substituted Ph, naphthyl, indolyl, indazolyl, thienyl, etc.; n = 1-2], useful for the treatment of depression (including but not limited to major depressive disorder, childhood depression and dysthymia), anxiety, panic disorder, post-traumatic stress disorder, premenstrual dysphoric disorder (also known as premenstrual syndrome), attention deficit disorder (with and without hyperactivity), obsessive compulsive disorder, social anxiety disorder, generalized anxiety disorder, obesity, eating disorders such as anorexia nervosa and bulimia nervosa, vasomotor flushing, cocaine and alc. addiction, sexual dysfunction and related illnesses, were prepared Thus, reacting [(2S)-8-methyl-2,3-dihydro[1,4]dioxino[2,3-f]quinolin-2-yl]methyl 4-bromobenzenesulfonate with 3-chlorophenylpiperazine.HCl in the presence of EtN(iso-Pr)2 in DMSO afforded 68% (2S)-2-{[4-(3-chlorophenyl)piperazin-

1-yl]methyl}-8-methyl-2,3-dihydro[1,4]dioxino[2,3-f]quinoline. The exemplified compds. I were tested for 5-HT transporter affinity, 5-HT_{1A} receptor affinity, and antagonistic activity at 5-HT_{1A} receptors and biol. data were given. The pharmaceutical composition comprising the compound I is claimed.

IT 676130-75-9P 676130-76-0P 676130-77-1P
 676130-78-2P 676130-79-3P 676130-80-6P
 676130-81-7P 676130-82-8P 676130-83-9P
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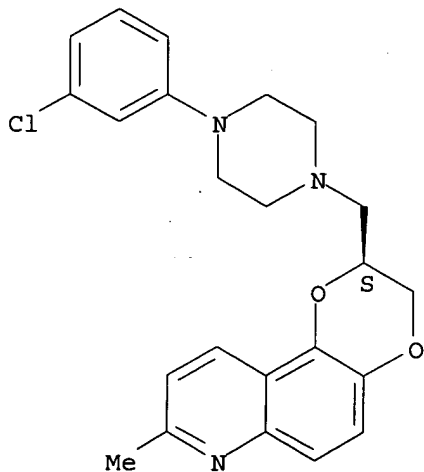
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of antidepressant arylpiperazine derivs. of heterocycle-fused benzodioxans as serotonin reuptake inhibitors and 5-HT_{1A} receptor antagonists)

RN 676130-75-9 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(3-chlorophenyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

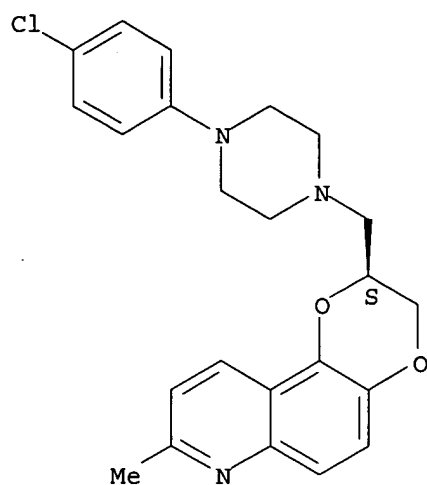


RN 676130-76-0 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(4-chlorophenyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

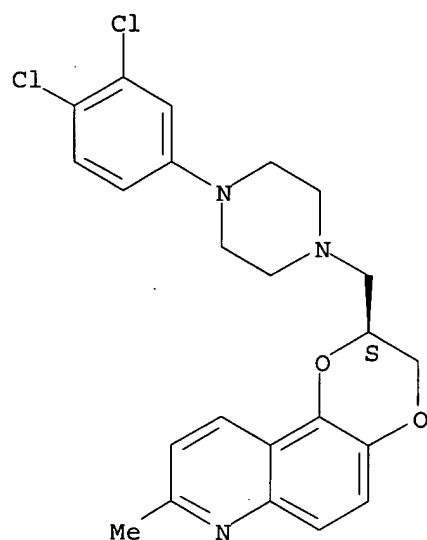
10/659537



RN 676130-77-1 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(3,4-dichlorophenyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 676130-78-2 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(3,4-dichlorophenyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)-, (2E)-2-butenedioate (2:1) (9CI) (CA INDEX NAME)

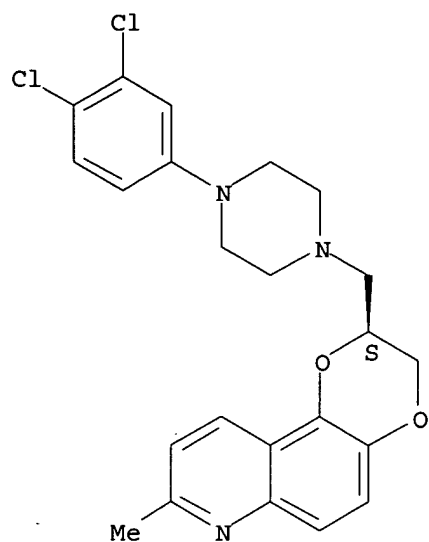
CM 1

CRN 676130-77-1

CMF C23 H23 Cl2 N3 O2

Absolute stereochemistry.

10/659537

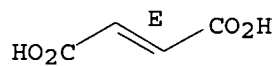


CM 2

CRN 110-17-8

CMF C4 H4 O4

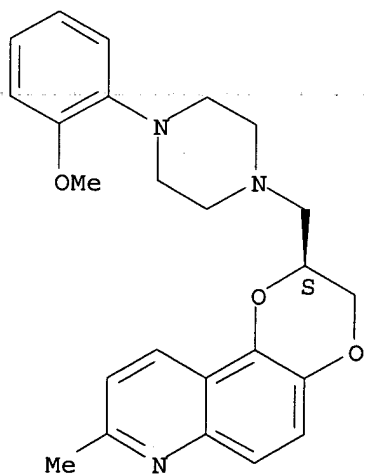
Double bond geometry as shown.



RN 676130-79-3 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

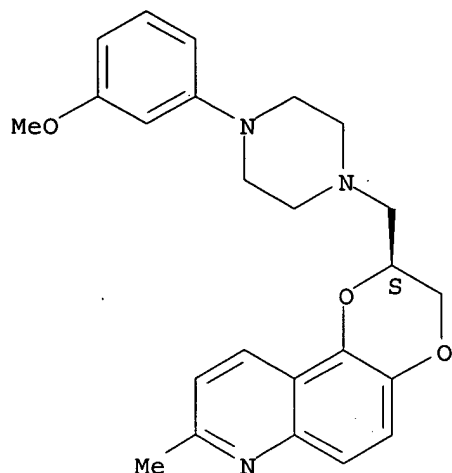


RN 676130-80-6 CAPLUS

10/659537

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-2-[[4-(3-methoxyphenyl)-1-piperazinyl]methyl]-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

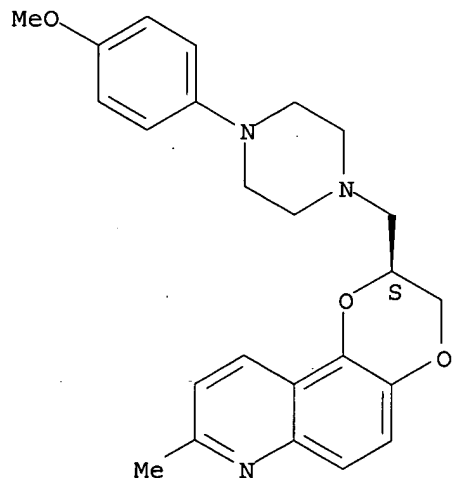
Absolute stereochemistry.



RN 676130-81-7 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-2-[[4-(4-methoxyphenyl)-1-piperazinyl]methyl]-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

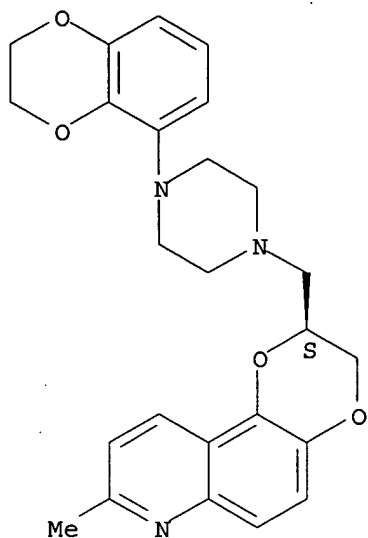


RN 676130-82-8 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(2,3-dihydro-1,4-benzodioxin-5-yl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/659537



RN 676130-83-9 CAPLUS

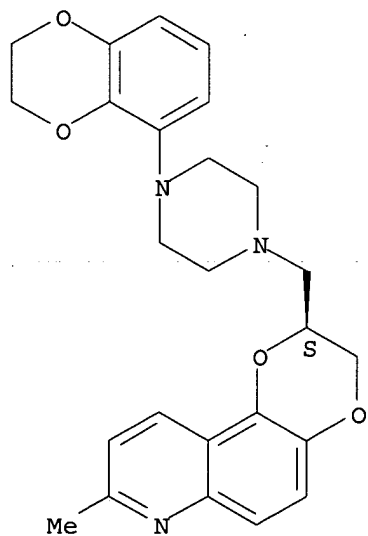
CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(2,3-dihydro-1,4-benzodioxin-5-yl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)-, (2E)-2-butenedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 676130-82-8

CMF C25 H27 N3 O4

Absolute stereochemistry.



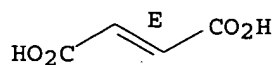
CM 2

CRN 110-17-8

CMF C4 H4 O4

10/659537

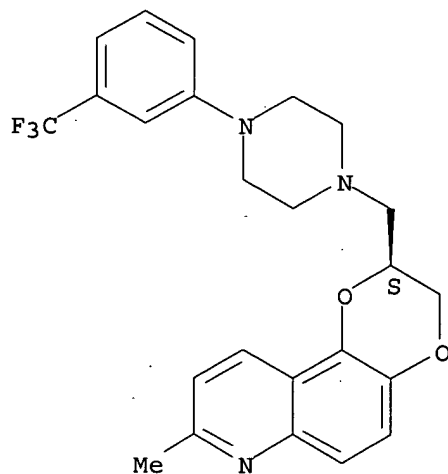
Double bond geometry as shown.



RN 676130-84-0 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

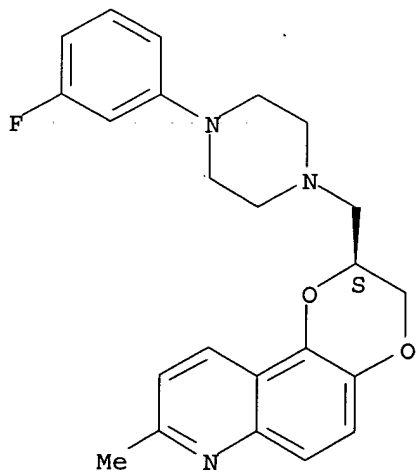
Absolute stereochemistry.



RN 676130-85-1 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(3-fluorophenyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



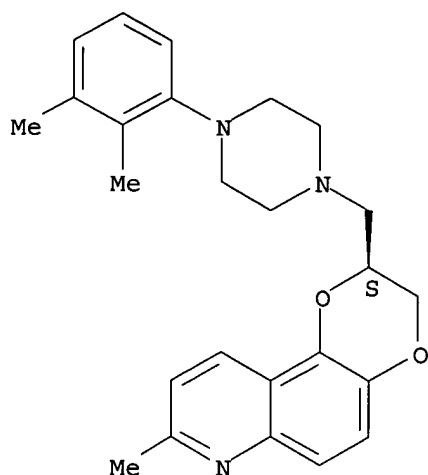
RN 676130-86-2 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(2,3-dimethylphenyl)-1-

10/659537

piperazinyl)methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

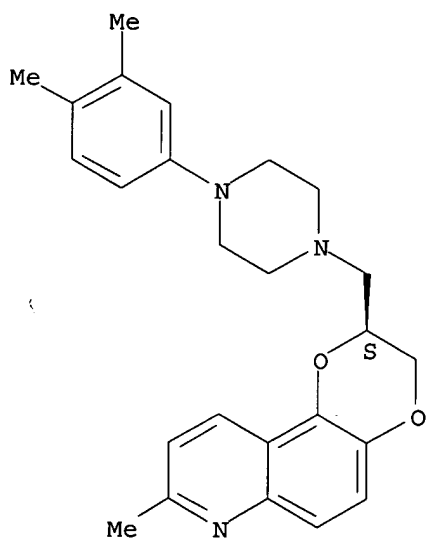
Absolute stereochemistry.



RN 676130-87-3 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(3,4-dimethylphenyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

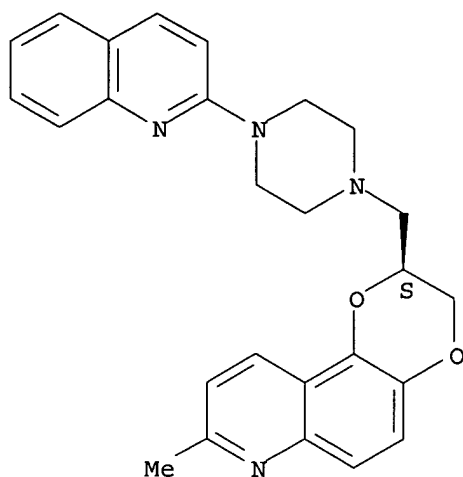


RN 676130-88-4 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-(2-quinolinyl)-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

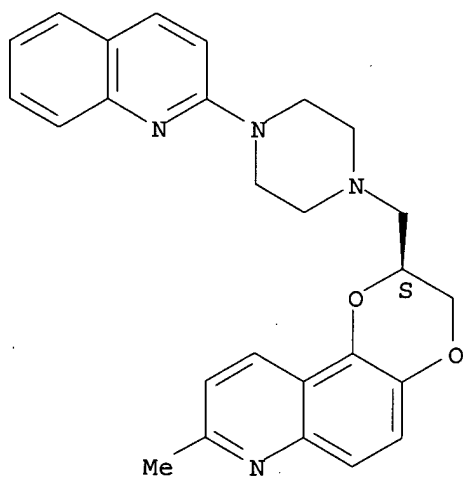
10/659537



RN 676130-89-5 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-(2-quinolinyl)-1-piperazinyl]methyl]-, tetrahydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



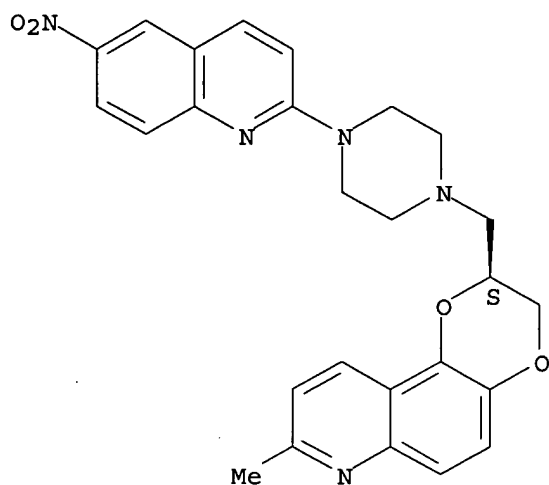
●4 HCl

RN 676130-90-8 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-(6-nitro-2-quinolinyl)-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

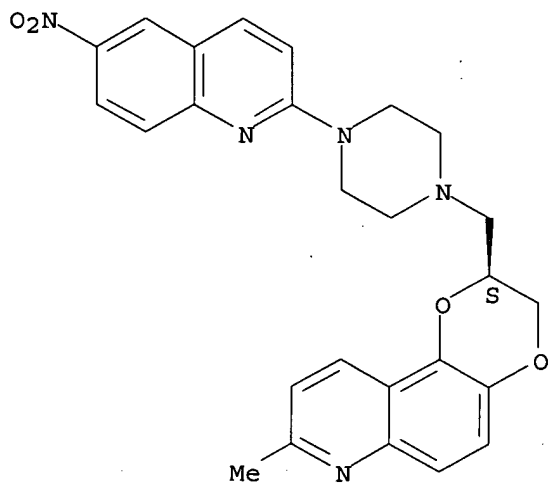
10/659537



RN 676130-91-9 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-(6-nitro-2-quinolinyl)-1-piperazinyl]methyl]-, hydrochloride (4:11), (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



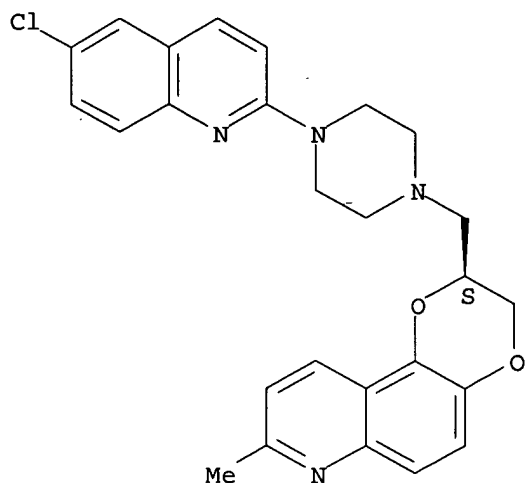
●11/4 HCl

RN 676130-92-0 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(6-chloro-2-quinolinyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

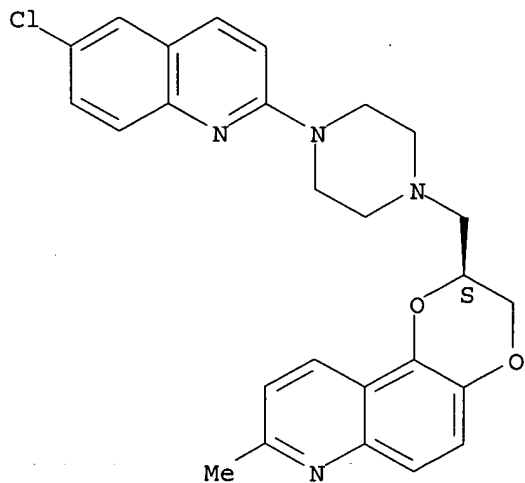
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RN 676130-93-1 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(6-chloro-2-quinolinyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, tetrahydrochloride, (2S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



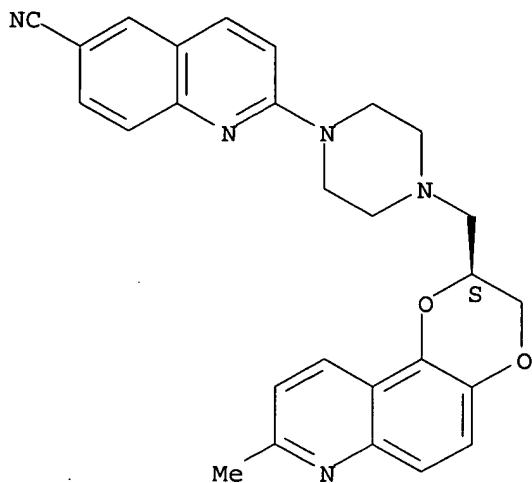
●4 HCl

RN 676130-94-2 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[2,3-dihydro-8-methyl-1,4-dioxino[2,3-f]quinolin-2-yl]methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

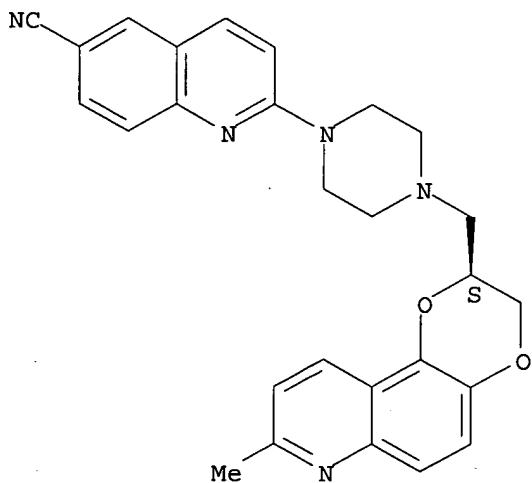
10/659537



RN 676130-95-3 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(2S)-2,3-dihydro-8-methyl-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]-, trihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



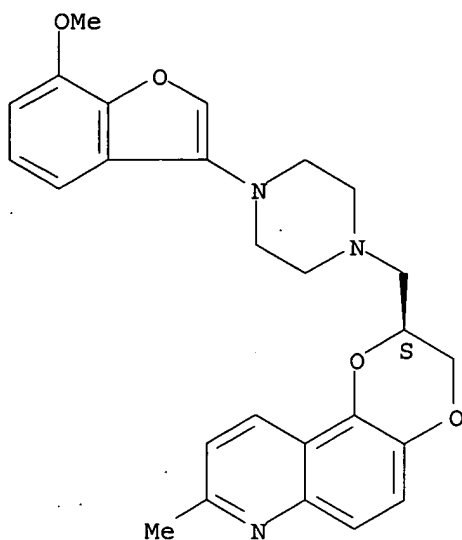
● 3 HCl

RN 676130-96-4 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-2-[[4-(7-methoxy-3-benzofuranyl)-1-piperazinyl)methyl]-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

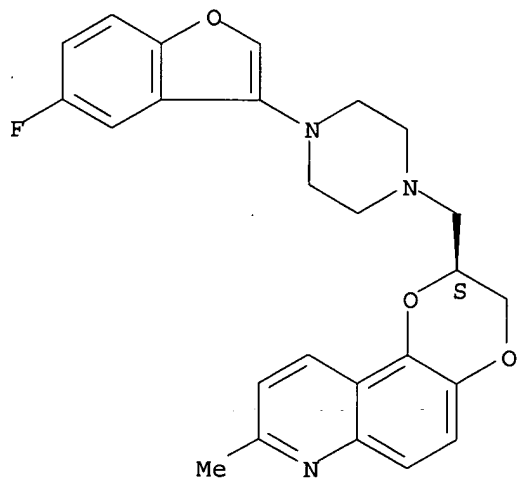
Absolute stereochemistry.

10/659537



RN 676130-97-5 CAPLUS
CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(5-fluoro-3-benzofuranyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, hydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

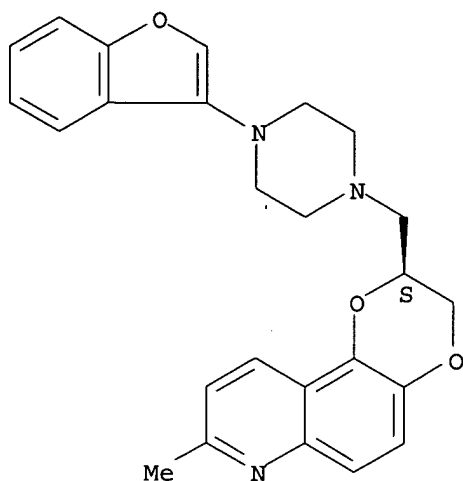


●x HCl

RN 676130-98-6 CAPLUS
CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(3-benzofuranyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

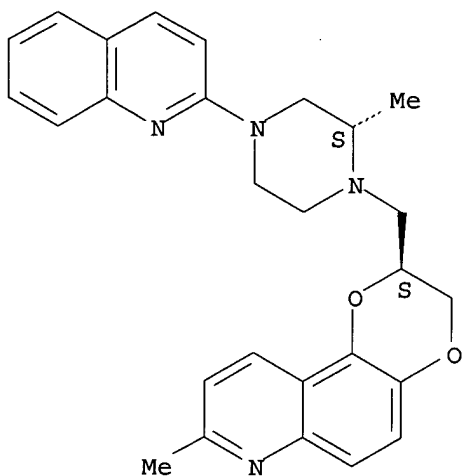
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RN 676130-99-7 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[[(2S)-2-methyl-4-(2-quinolinyl)-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

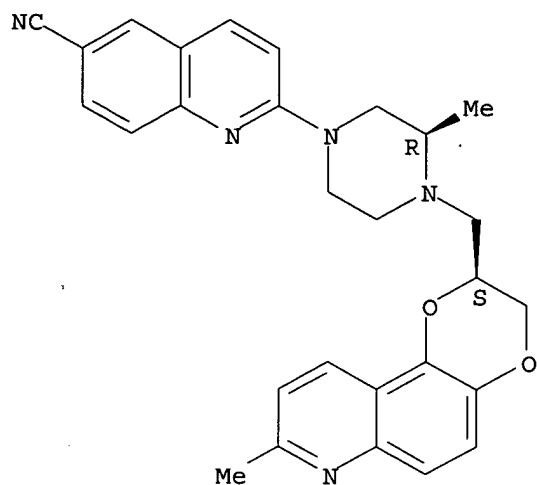


RN 676131-00-3 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[(3R)-4-[[[(2S)-2,3-dihydro-8-methyl-1,4-dioxino[2,3-f]quinolin-2-yl]methyl]-3-methyl-1-piperazinyl]-, (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

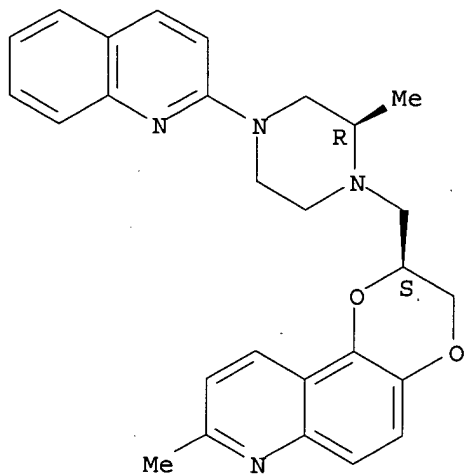
10/659537



RN 676131-01-4 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[[(2R)-2-methyl-4-(2-quinolinyl)-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

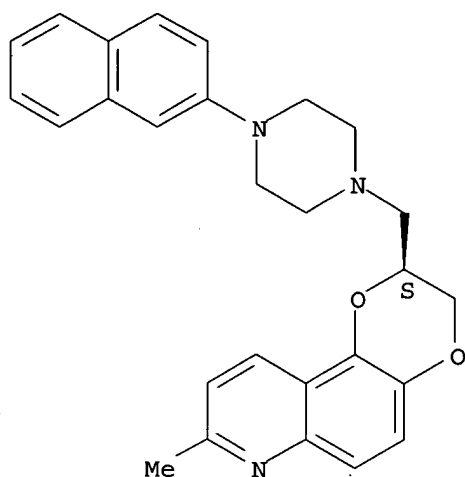


RN 676131-02-5 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-(2-naphthalenyl)-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

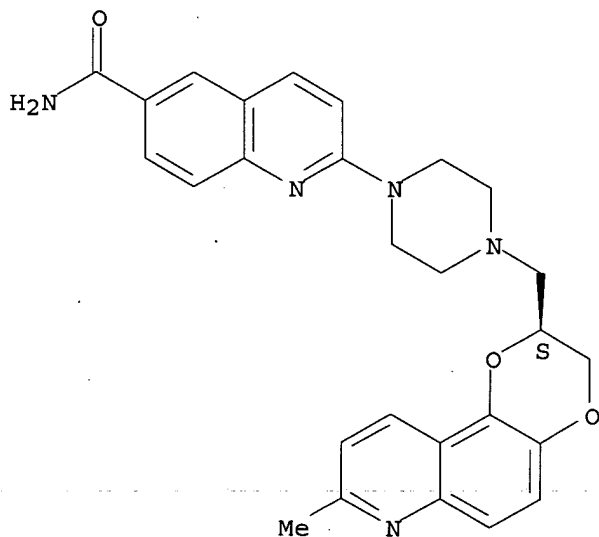
10/659537



RN 676131-03-6 CAPLUS

CN 6-Quinolinecarboxamide, 2-[4-[[[(2S)-2,3-dihydro-8-methyl-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

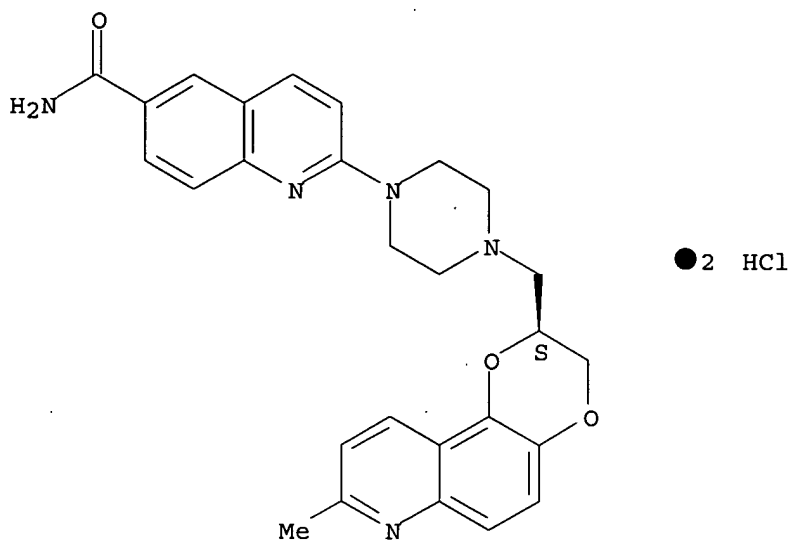


RN 676131-04-7 CAPLUS

CN 6-Quinolinecarboxamide, 2-[4-[[[(2S)-2,3-dihydro-8-methyl-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

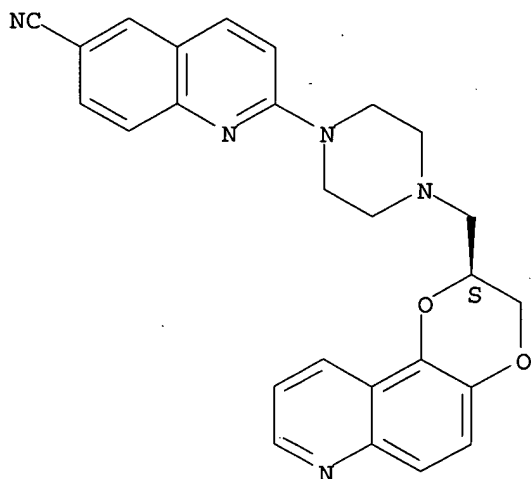
10/659537



RN 676131-05-8 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(2S)-2,3-dihydro-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

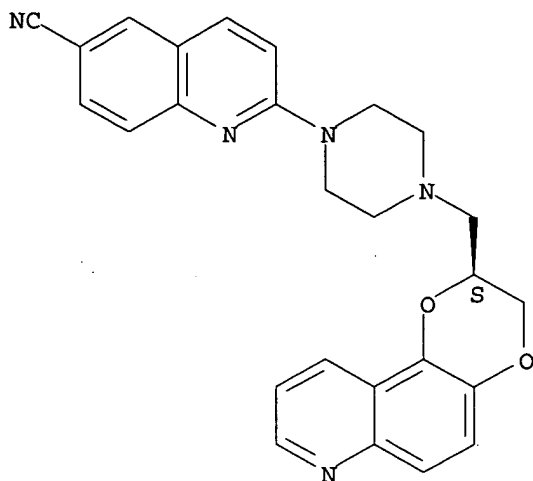


RN 676131-06-9 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(2S)-2,3-dihydro-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]-, trihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/659537

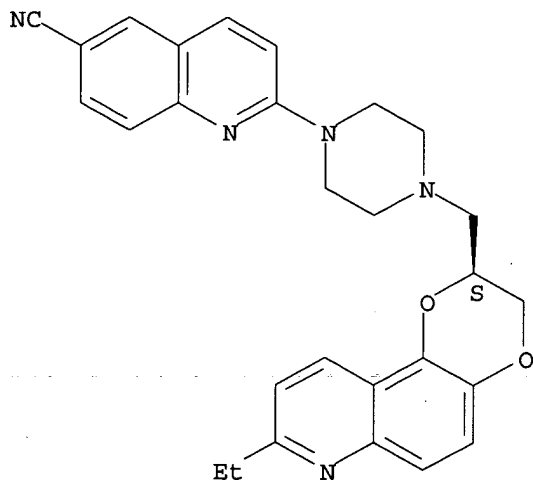


● 3 HCl

RN 676131-07-0 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(2S)-8-ethyl-2,3-dihydro-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

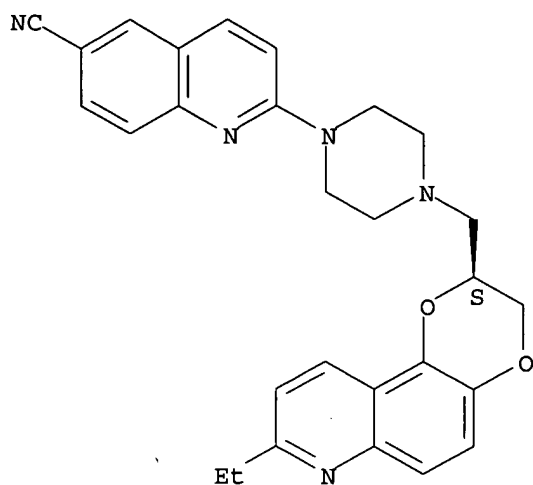


RN 676131-08-1 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(2S)-8-ethyl-2,3-dihydro-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]-, trihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/659537

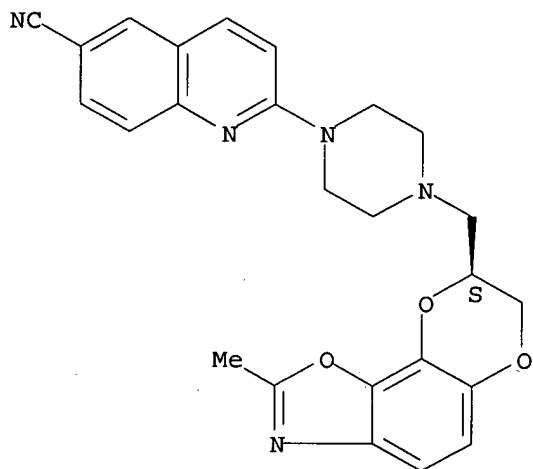


● 3 HCl

RN 676131-09-2 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(8S)-7,8-dihydro-2-methyl[1,4]dioxino[2,3-g]benzoxazol-8-yl]methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

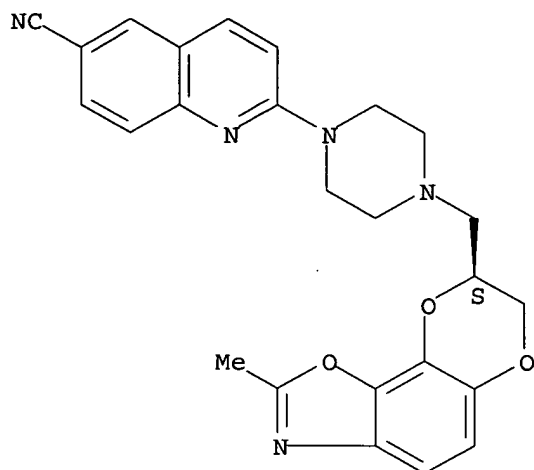


RN 676131-10-5 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(8S)-7,8-dihydro-2-methyl[1,4]dioxino[2,3-g]benzoxazol-8-yl]methyl]-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/659537

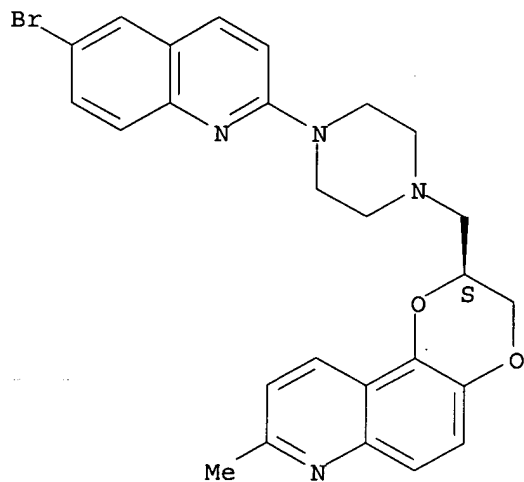


● 2 HCl

RN 676131-11-6 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(6-bromo-2-quinolinyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

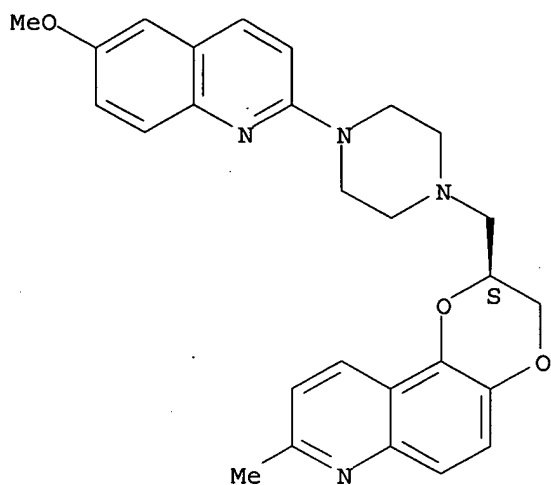


RN 676131-12-7 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-2-[[4-(6-methoxy-2-quinolinyl)-1-piperazinyl]methyl]-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

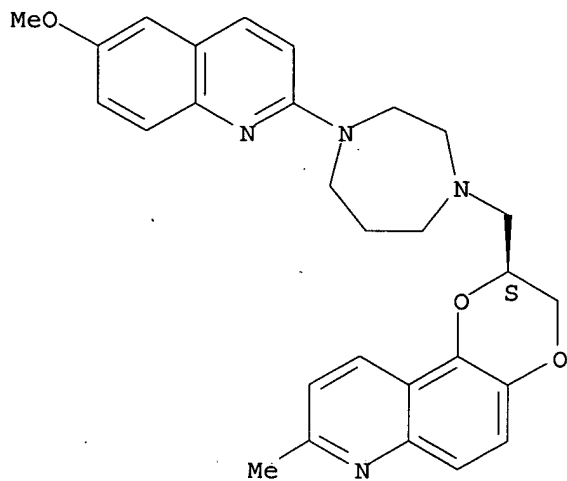
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RN 676131-13-8 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[hexahydro-4-(6-methoxy-2-quinolinyl)-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

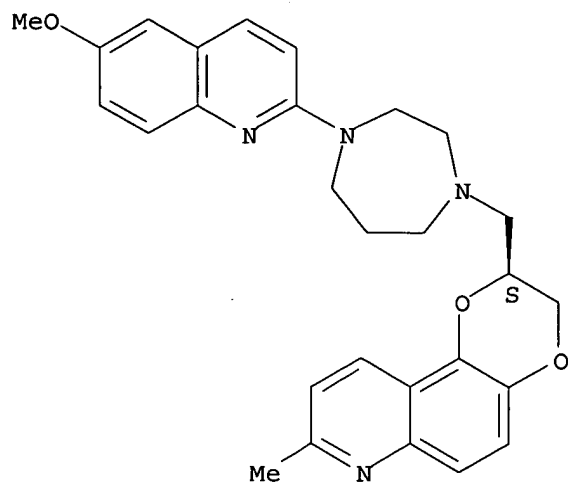


RN 676131-14-9 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[hexahydro-4-(6-methoxy-2-quinolinyl)-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl-, trihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/659537

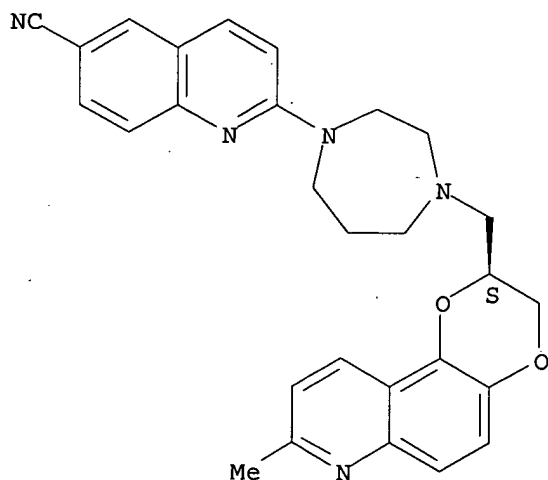


●₃ HCl

RN 676131-15-0 CAPLUS

CN 6-Quinolines carbonitrile, 2-[4-[[[(2S)-2,3-dihydro-8-methyl-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]hexahydro-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

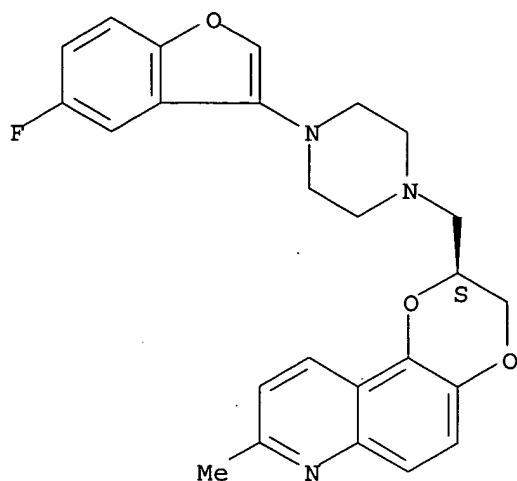


RN 676131-32-1 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(5-fluoro-3-benzofuranyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

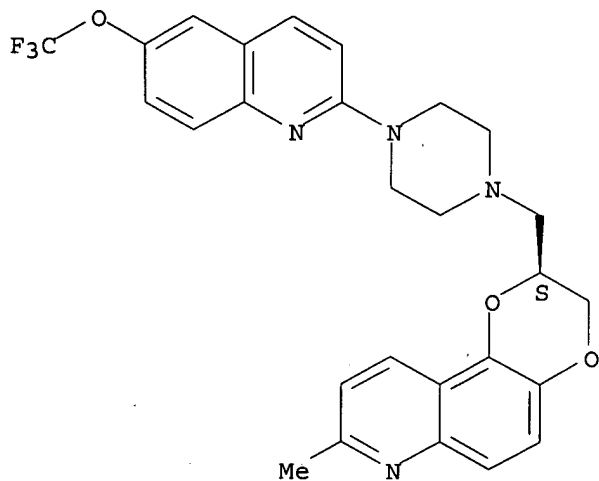
10/659537



RN 676131-33-2 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-[6-(trifluoromethoxy)-2-quinolinyl]-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

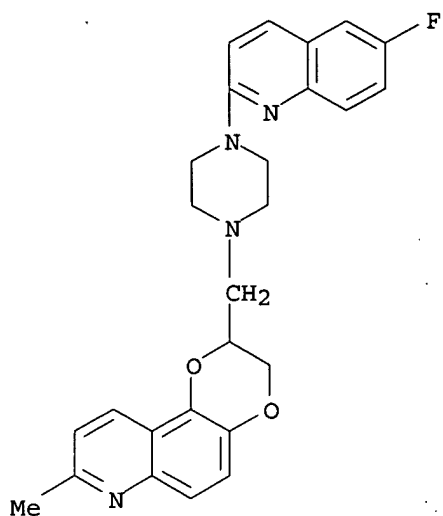
Absolute stereochemistry.



RN 676131-34-3 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(6-fluoro-2-quinolinyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl- (9CI) (CA INDEX NAME)

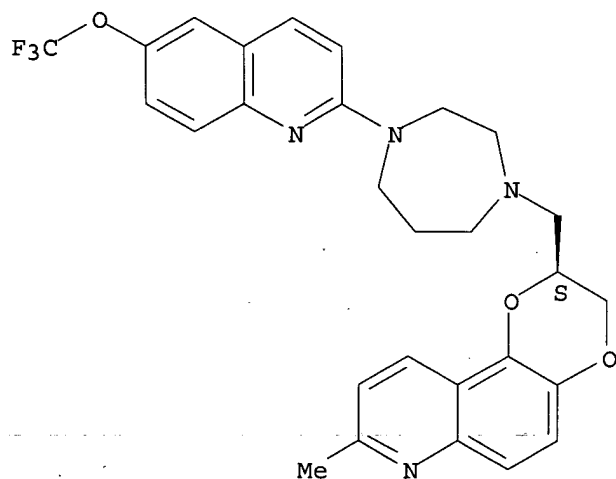
10/659537



RN 676131-35-4 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[hexahydro-4-[6-(trifluoromethoxy)-2-quinolinyl]-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

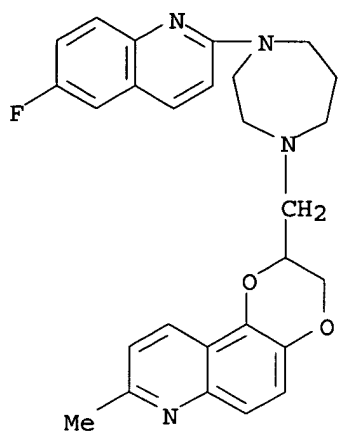
Absolute stereochemistry.



RN 676131-36-5 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(6-fluoro-2-quinolinyl)hexahydro-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl- (9CI) (CA INDEX NAME)

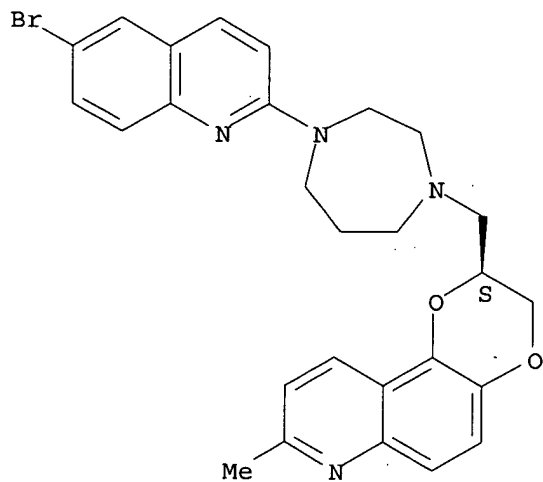
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RN 676131-37-6 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(6-bromo-2-quinolinyl)hexahydro-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

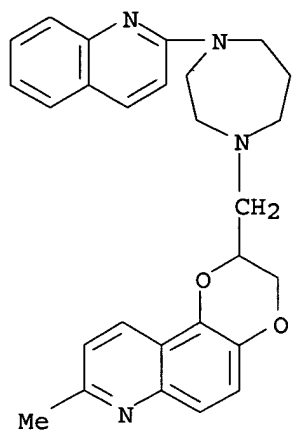
Absolute stereochemistry.



RN 676131-38-7 CAPLUS

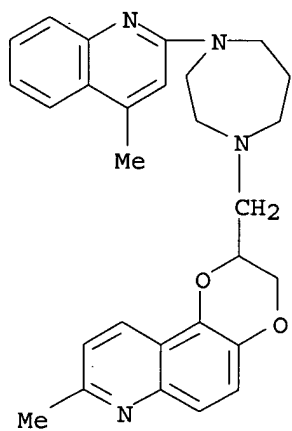
CN 1,4-Dioxino[2,3-f]quinoline, 2-[[hexahydro-4-(2-quinolinyl)-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl- (9CI) (CA INDEX NAME)

10/659537



RN 676131-39-8 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[hexahydro-4-(4-methyl-2-quinolinyl)-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl- (9CI) (CA INDEX NAME)



10/659537

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:252515 CAPLUS
DN 140:287410
TI Preparation of antidepressant arylpiperazine derivatives of
heterocycle-fused benzodioxans
IN Evrard, Deborah A.; Zhou, Dahui; Stack, Gary Paul; Venkatesan, Arenapakam
Madumbai; Failli, Amedeo A.; Croce, Susan Christman
PA Wyeth, John, and Brother Ltd., USA
SO PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

PATENT NO. KIND DATE APPLICATION NO. DATE

PI WO 2004024731 A1 20040325 WO 2003-US28453 20030911

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM,
PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
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KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
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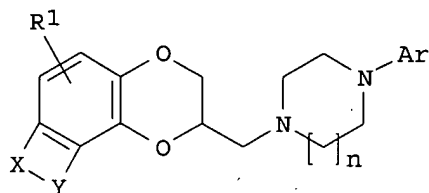
US 2004142926 A1 20040722 US 2003-659537 20030910

PRAI US 2002-410082P P 20020912

US 2003-659537 A 20030910

OS MARPAT 140:287410

GI



AB The title compds. [R1 = H, halo, CN, carboxamido, etc.; XY = N:CR2CR3:N, N:CR2CR4:CH, N:CR2N:CH, N:CR2O, NHCR5:CH; R2, R3 = H, halo, NH2, mono-or dialkylamino, alkyl; R4 = H, alkyl; R5 = H, halo, CF3, pentafluoroethyl, alkyl; Ar = (un)substituted Ph, naphthyl, indoleyl, indazolyl, thienyl, etc.; n = 1-2], useful for the treatment of depression (including but not limited to major depressive disorder, childhood depression and dysthymia), anxiety, panic disorder, post-traumatic stress disorder, premenstrual dysphoric disorder (also known as premenstrual syndrome), attention deficit disorder (with and without hyperactivity), obsessive compulsive disorder, social anxiety disorder, generalized anxiety disorder, obesity, eating disorders such as anorexia nervosa and bulimia nervosa, vasomotor flushing, cocaine and alc. addiction, sexual dysfunction and related illnesses, were prepared Thus, reacting [(2S)-8-methyl-2,3-dihydro[1,4]dioxino[2,3-f]quinolin-2-yl)methyl 4-bromobenzenesulfonate with 3-chlorophenylpiperazine.HCl in the presence of EtN(iso-Pr)2 in DMSO afforded 68% (2S)-2-{[4-(3-chlorophenyl)piperazin-1-yl)methyl}-8-methyl-2,3-dihydro[1,4]dioxino[2,3-f]quinoline. The exemplified compds. I were

tested for 5-HT transporter affinity, 5-HT_{1A} receptor affinity, and antagonistic activity at 5-HT_{1A} receptors and biol. data were given. The pharmaceutical composition comprising the compound I is claimed.

IT 676130-75-9P 676130-76-0P 676130-77-1P
 676130-78-2P 676130-79-3P 676130-80-6P
 676130-81-7P 676130-82-8P 676130-83-9P
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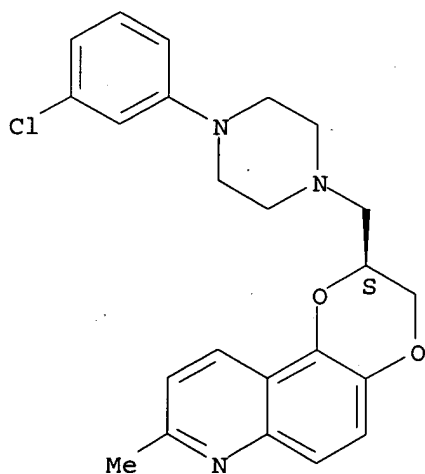
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of antidepressant arylpiperazine derivs. of heterocycle-fused benzodioxans as serotonin reuptake inhibitors and 5-HT_{1A} receptor antagonists)

RN 676130-75-9 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(3-chlorophenyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

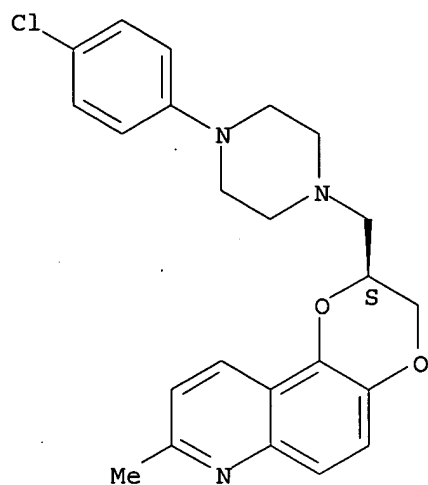


RN 676130-76-0 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(4-chlorophenyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

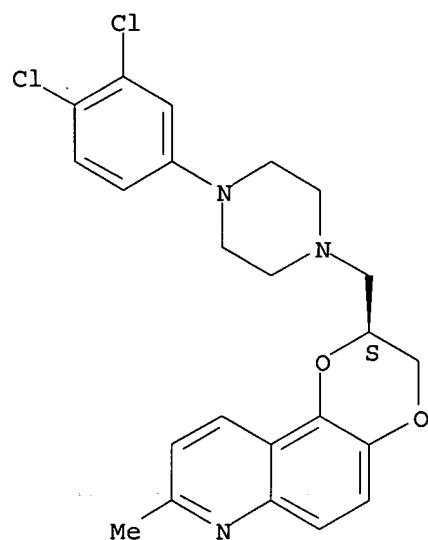
10/659537



RN 676130-77-1 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(3,4-dichlorophenyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 676130-78-2 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(3,4-dichlorophenyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)-, (2E)-2-butenedioate (2:1) (9CI) (CA INDEX NAME)

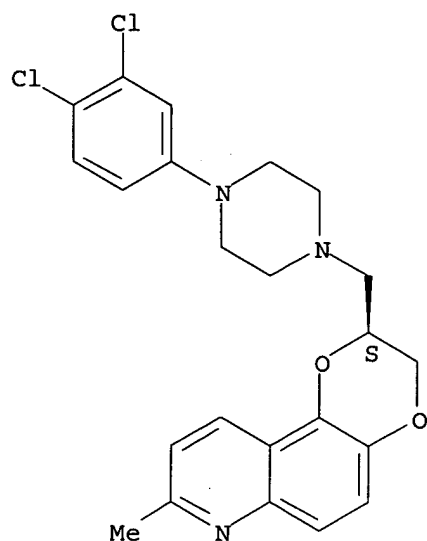
CM 1

CRN 676130-77-1

CMF C23 H23 Cl2 N3 O2

Absolute stereochemistry.

10/659537

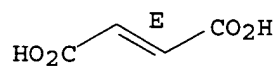


CM 2

CRN 110-17-8

CMF C4 H4 O4

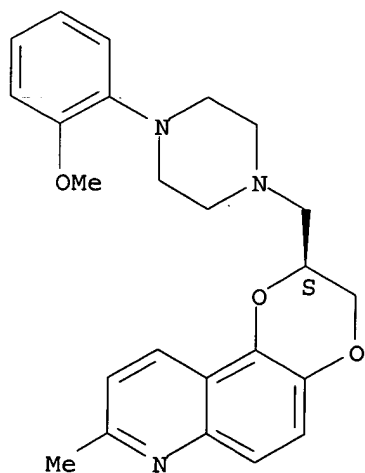
Double bond geometry as shown.



RN 676130-79-3 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-2-[[4-(2-methoxyphenyl)-1-piperazinyl]methyl]-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

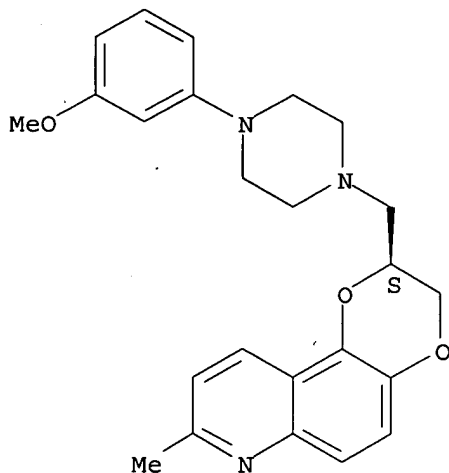


RN 676130-80-6 CAPLUS

10/659537

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-2-[[4-(3-methoxyphenyl)-1-piperazinyl]methyl]-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

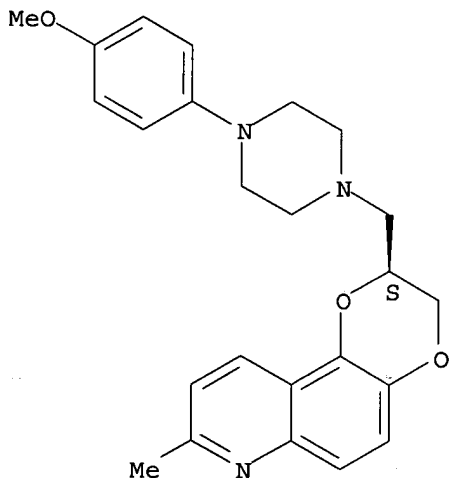
Absolute stereochemistry.



RN 676130-81-7 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-2-[[4-(4-methoxyphenyl)-1-piperazinyl]methyl]-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

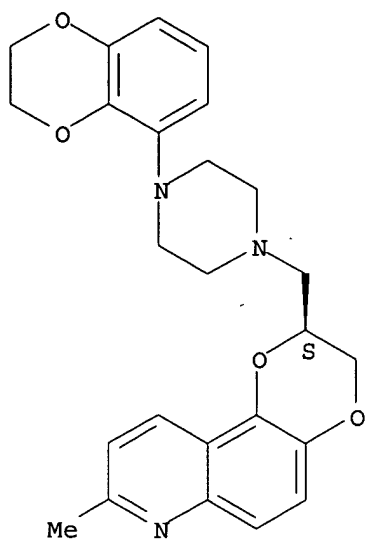


RN 676130-82-8 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(2,3-dihydro-1,4-benzodioxin-5-yl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/659537



RN 676130-83-9 CAPLUS

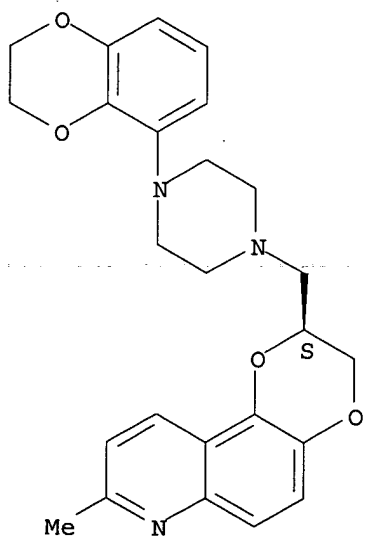
CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(2,3-dihydro-1,4-benzodioxin-5-yl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)-, (2E)-2-butenedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 676130-82-8

CMF C25 H27 N3 O4

Absolute stereochemistry.



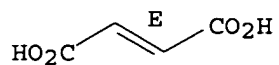
CM 2

CRN 110-17-8

CMF C4 H4 O4

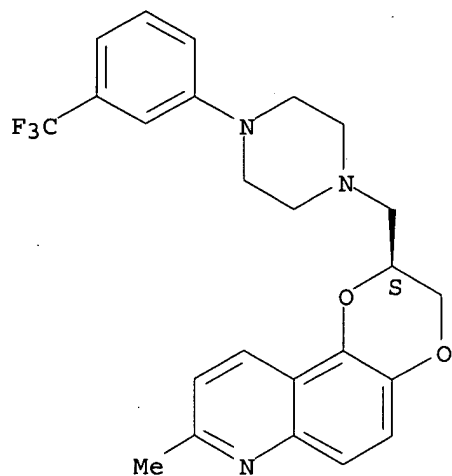
10/659537

Double bond geometry as shown.



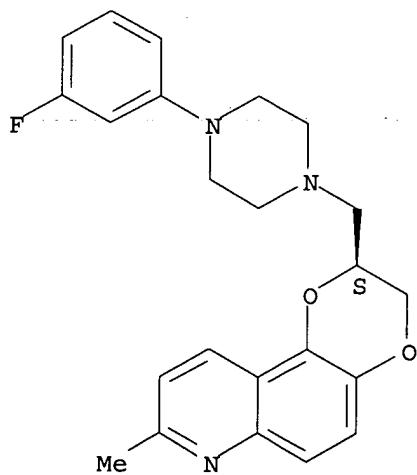
RN 676130-84-0 CAPLUS
CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-[3-(trifluoromethyl)phenyl]-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 676130-85-1 CAPLUS
CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(3-fluorophenyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

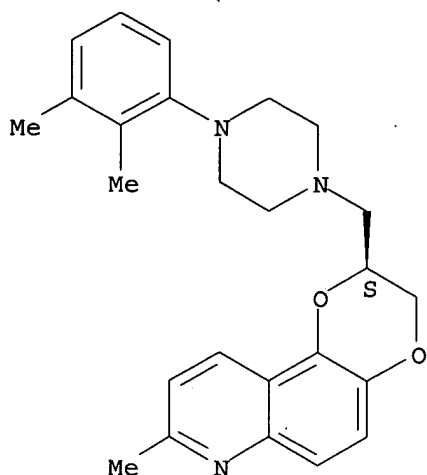


RN 676130-86-2 CAPLUS
CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(2,3-dimethylphenyl)-1-

10/659537

piperazinyl)methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

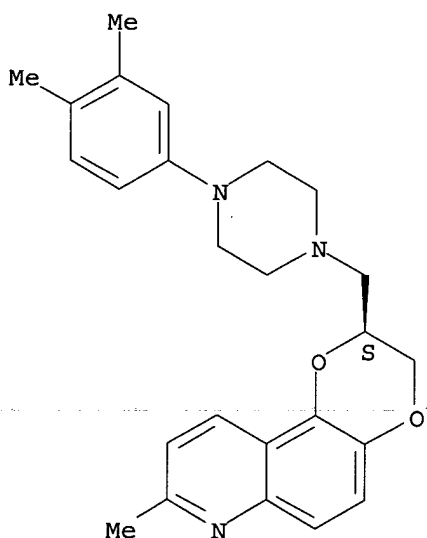
Absolute stereochemistry.



RN 676130-87-3 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(3,4-dimethylphenyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

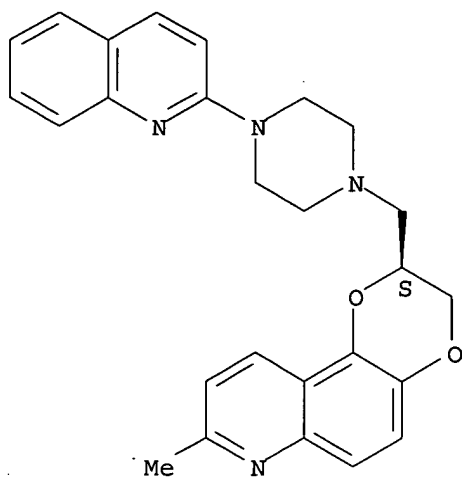


RN 676130-88-4 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-(2-quinolinyl)-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

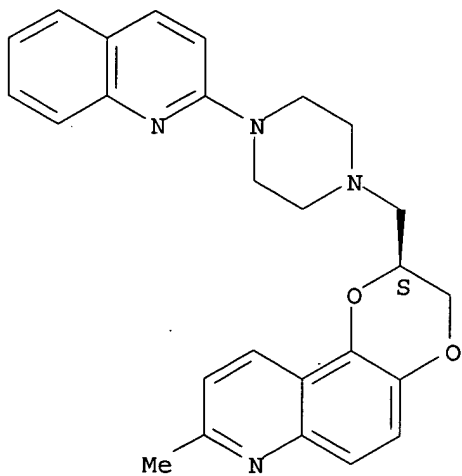
10/659537



RN 676130-89-5 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-(2-quinolinyl)-1-piperazinyl]methyl]-, tetrahydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



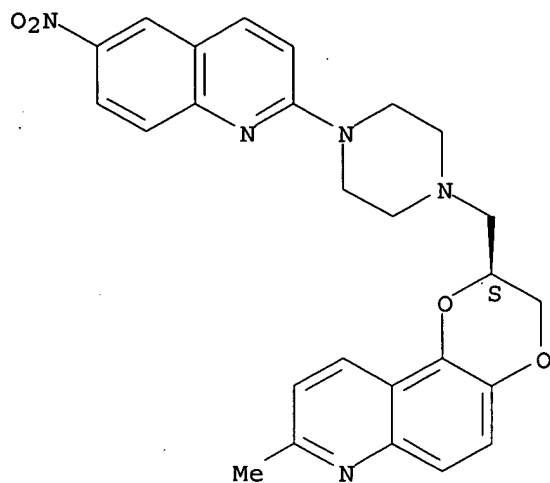
● 4 HCl

RN 676130-90-8 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-(6-nitro-2-quinolinyl)-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

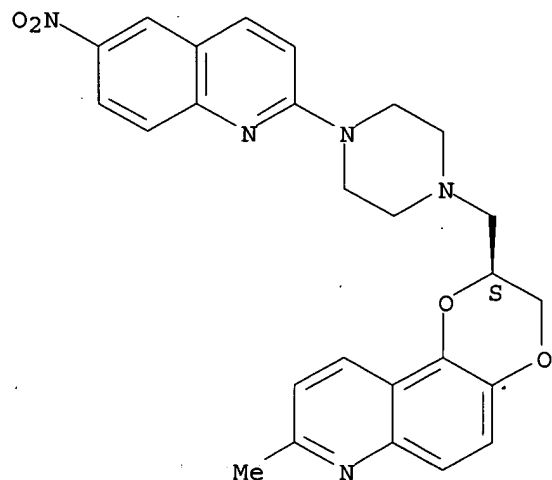
10/659537



RN 676130-91-9 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-(6-nitro-2-quinolinyl)-1-piperazinyl]methyl]-, hydrochloride (4:11), (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



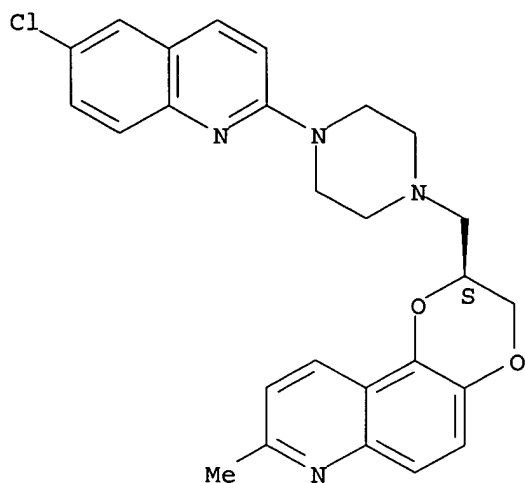
●11/4 HCl

RN 676130-92-0 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(6-chloro-2-quinolinyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

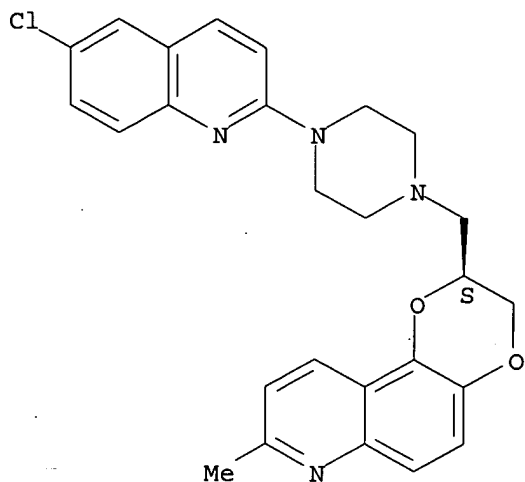
10/659537



RN 676130-93-1 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(6-chloro-2-quinolinyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, tetrahydrochloride, (2S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



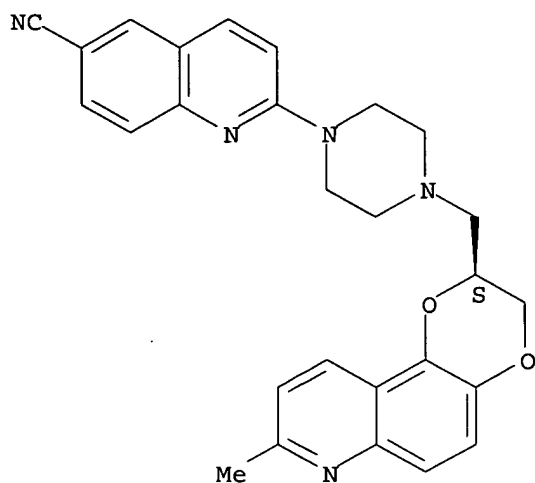
●4 HCl

RN 676130-94-2 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(2S)-2,3-dihydro-8-methyl-1,4-dioxino[2,3-f]quinolin-2-yl]methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

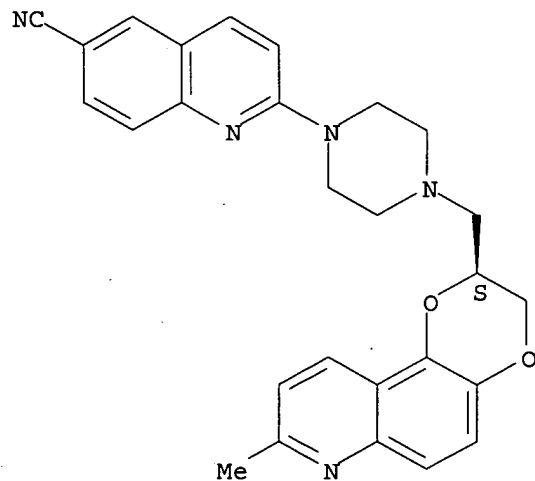
10/659537



RN 676130-95-3 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(2S)-2,3-dihydro-8-methyl-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]-, trihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



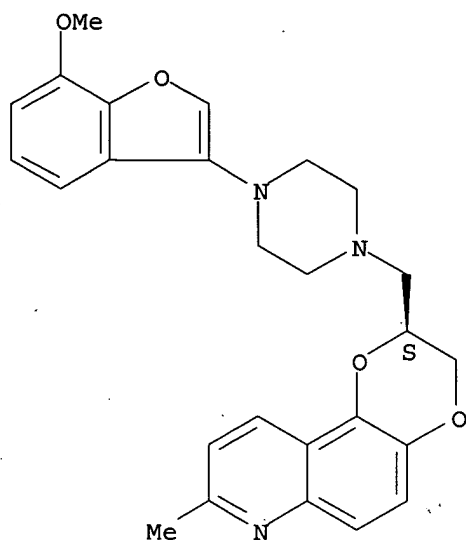
●3 HCl

RN 676130-96-4 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-2-[[4-(7-methoxy-3-benzofuranyl)-1-piperazinyl)methyl]-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

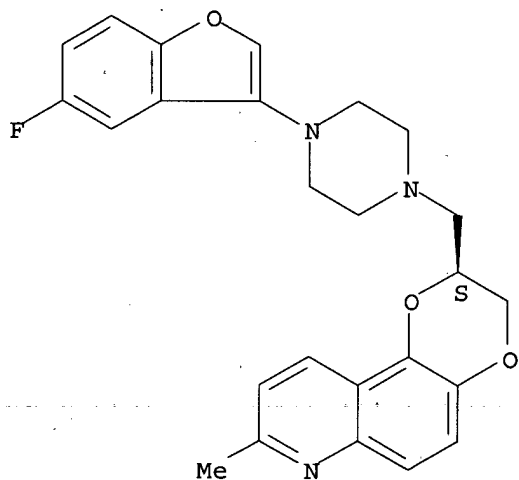
10/659537



RN 676130-97-5 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(5-fluoro-3-benzofuranyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, hydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



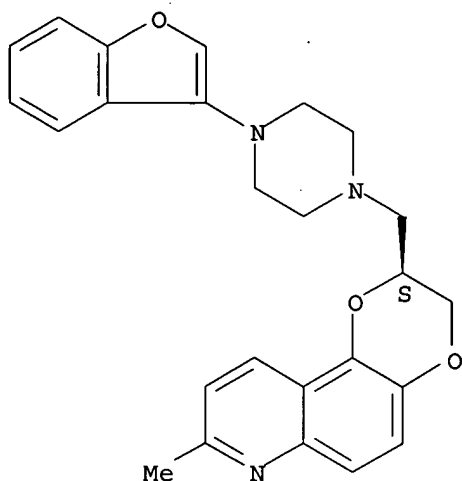
● x HCl

RN 676130-98-6 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(3-benzofuranyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

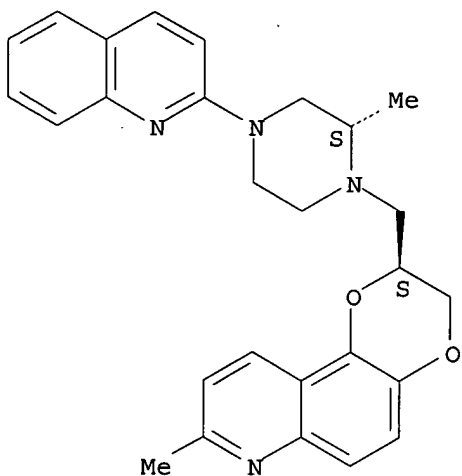
10/659537



RN 676130-99-7 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[2-(2-quinolinyl)-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

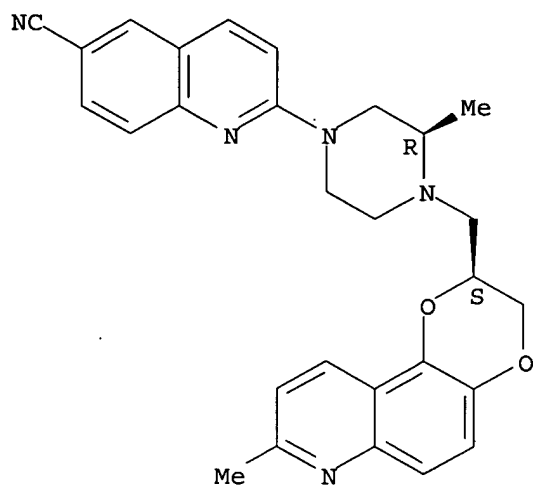


RN 676131-00-3 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[(3R)-4-[[2-(2,3-dihydro-8-methyl-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-3-methyl-1-piperazinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

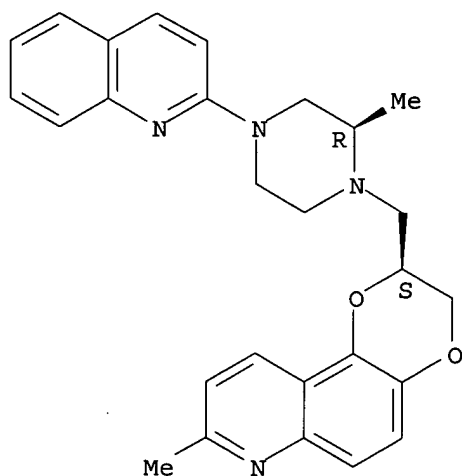
10/659537



RN 676131-01-4 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[[(2R)-2-methyl-4-(2-quinolinyl)-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

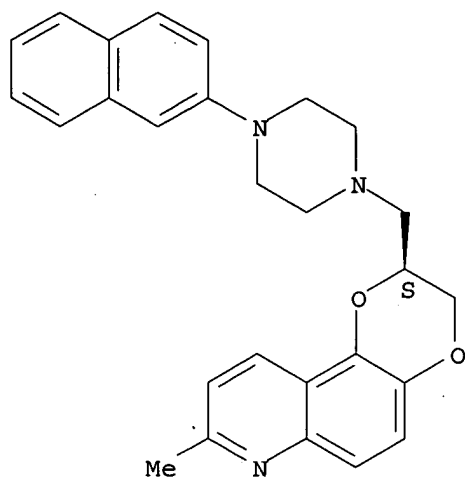


RN 676131-02-5 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-(2-naphthalenyl)-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

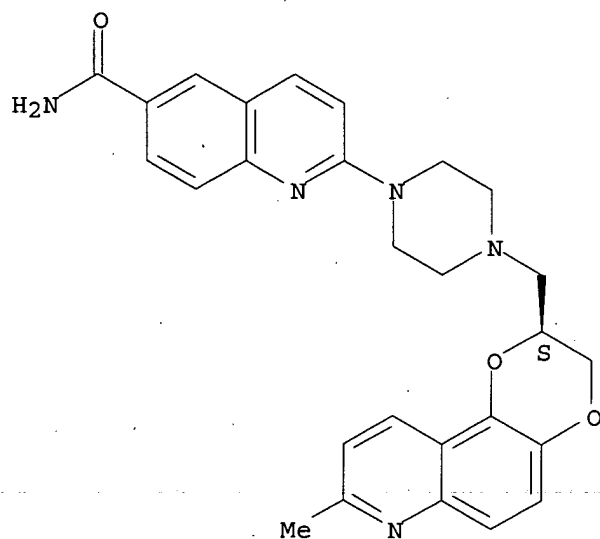
10/659537



RN 676131-03-6 CAPLUS

CN 6-Quinolinecarboxamide, 2-[4-[[[(2S)-2,3-dihydro-8-methyl-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

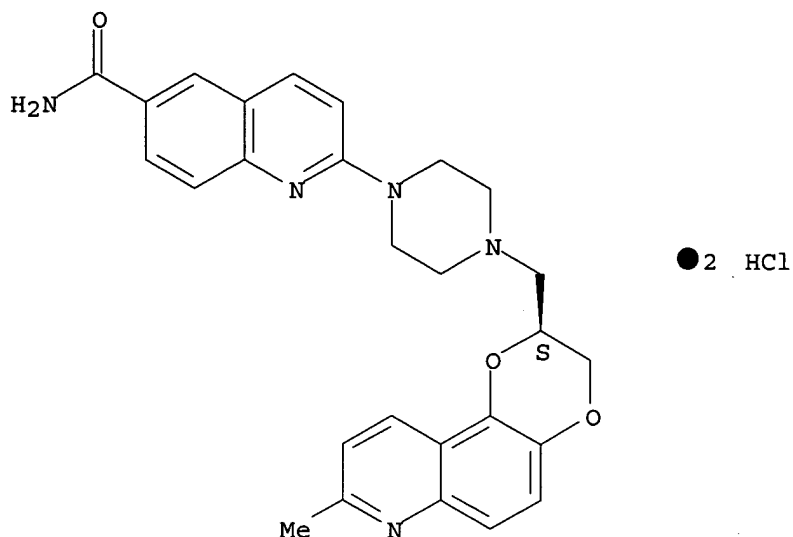


RN 676131-04-7 CAPLUS

CN 6-Quinolinecarboxamide, 2-[4-[[[(2S)-2,3-dihydro-8-methyl-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

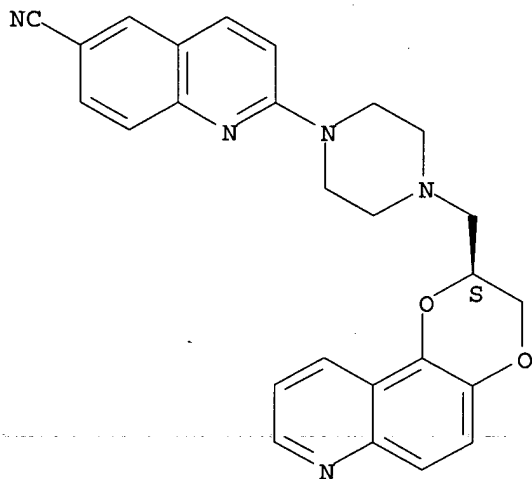
10/659537



RN 676131-05-8 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(2S)-2,3-dihydro-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

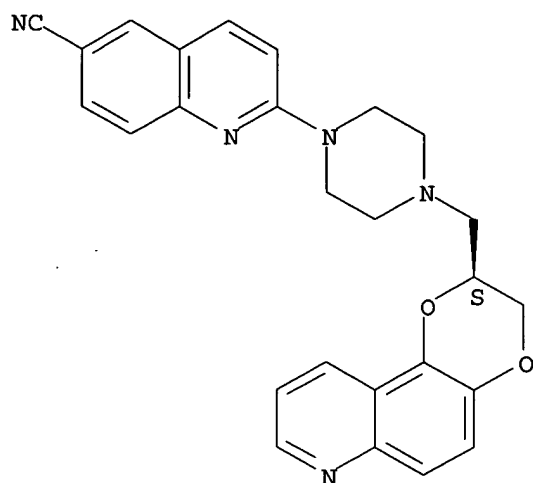


RN 676131-06-9 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(2S)-2,3-dihydro-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]-, trihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/659537

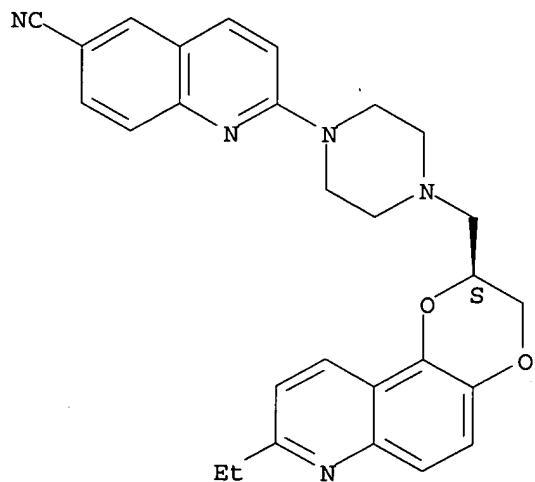


● 3 HCl

RN 676131-07-0 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(2S)-8-ethyl-2,3-dihydro-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

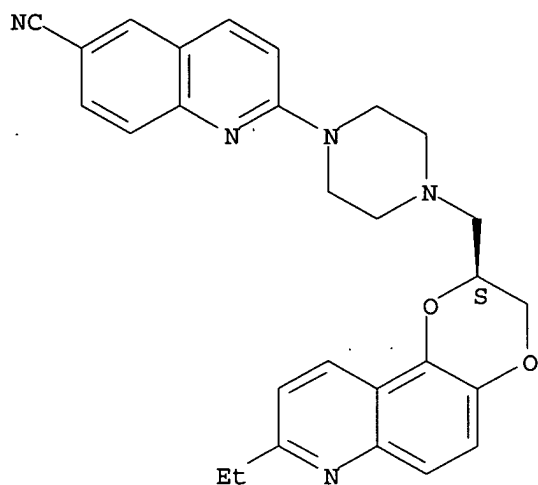


RN 676131-08-1 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(2S)-8-ethyl-2,3-dihydro-1,4-dioxino[2,3-f]quinolin-2-yl)methyl]-1-piperazinyl]-, trihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/659537

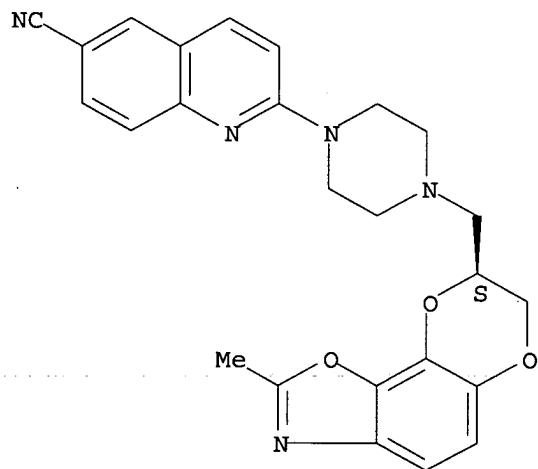


● 3 HCl

RN 676131-09-2 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(8S)-7,8-dihydro-2-methyl[1,4]dioxino[2,3-g]benzoxazol-8-yl]methyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

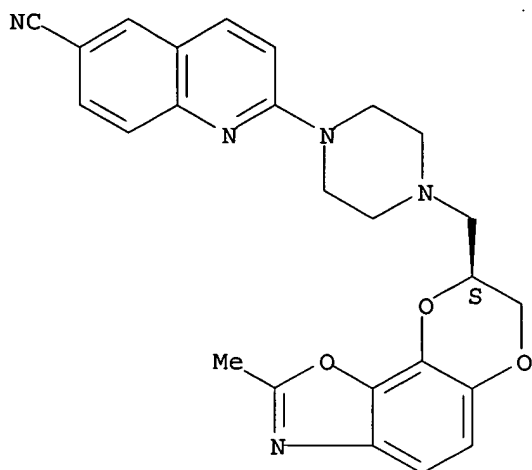


RN 676131-10-5 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[[(8S)-7,8-dihydro-2-methyl[1,4]dioxino[2,3-g]benzoxazol-8-yl]methyl]-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

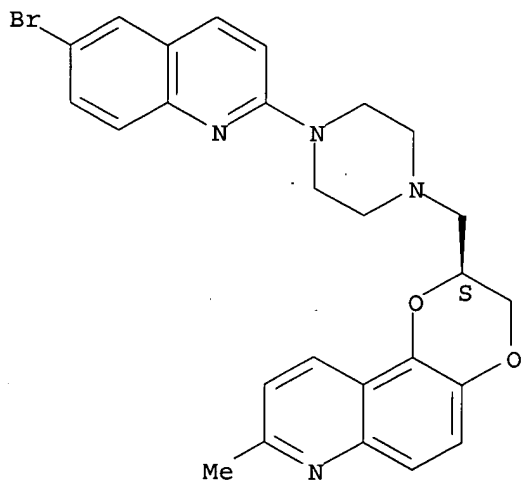
10/659537



● 2 HCl

RN 676131-11-6 CAPLUS
CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(6-bromo-2-quinolinyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

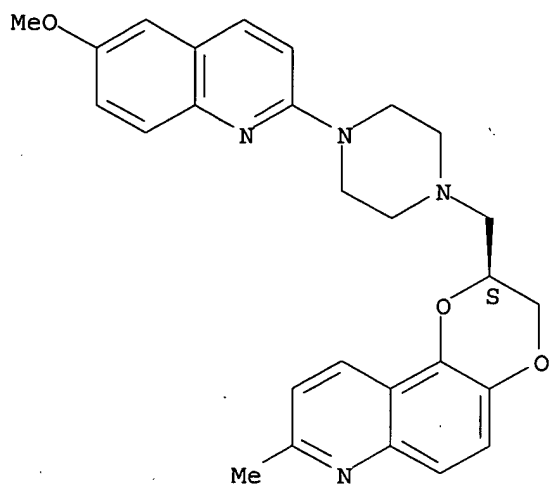
Absolute stereochemistry.



RN 676131-12-7 CAPLUS
CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-2-[[4-(6-methoxy-2-quinolinyl)-1-piperazinyl]methyl]-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

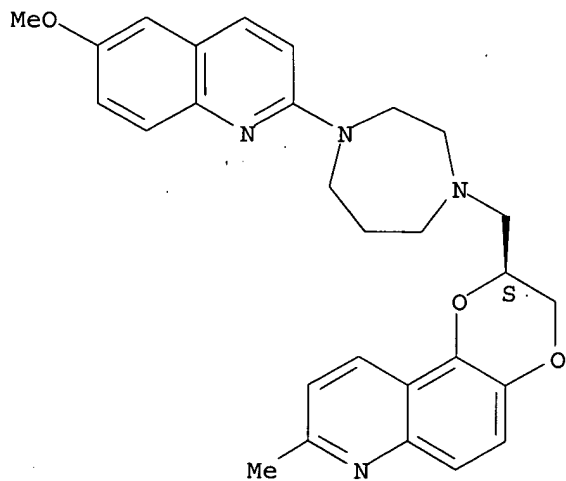
10/659537



RN 676131-13-8 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[hexahydro-4-(6-methoxy-2-quinolinyl)-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

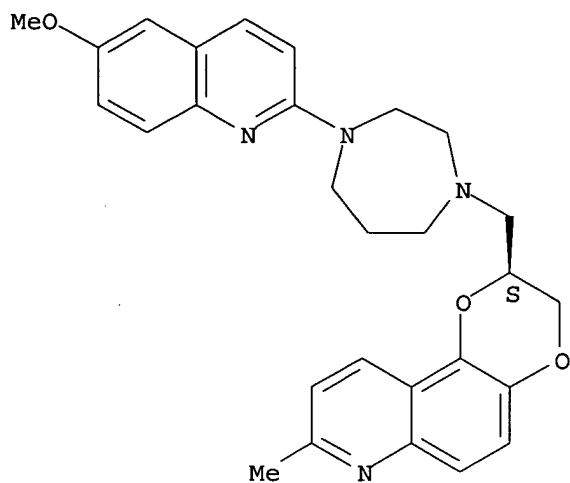


RN 676131-14-9 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[hexahydro-4-(6-methoxy-2-quinolinyl)-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl-, trihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/659537

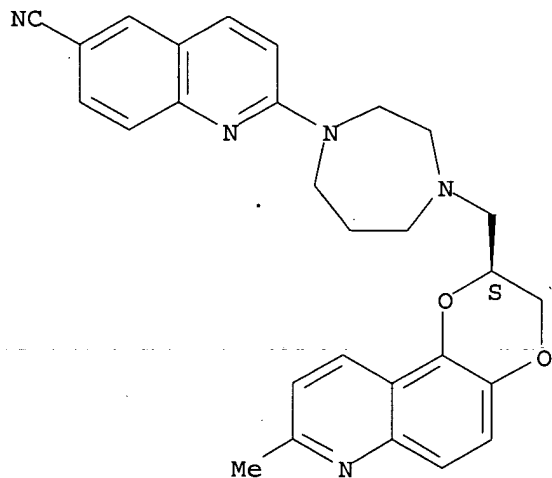


● 3 HCl

RN 676131-15-0 CAPLUS

CN 6-Quinolinecarbonitrile, 2-[4-[[2,3-dihydro-8-methyl-1,4-dioxino[2,3-f]quinolin-2-yl]methyl]hexahydro-1H-1,4-diazepin-1-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

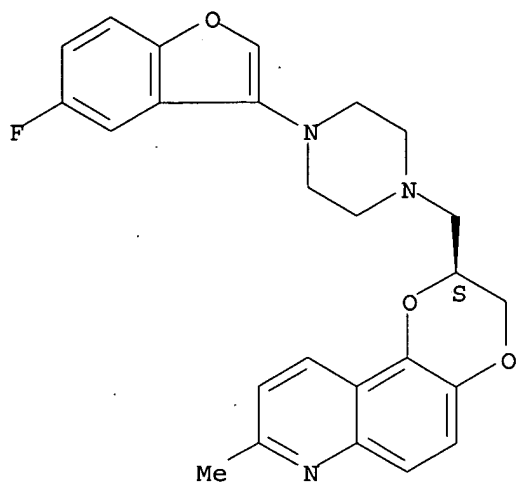


RN 676131-32-1 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[4-(5-fluoro-3-benzofuranyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

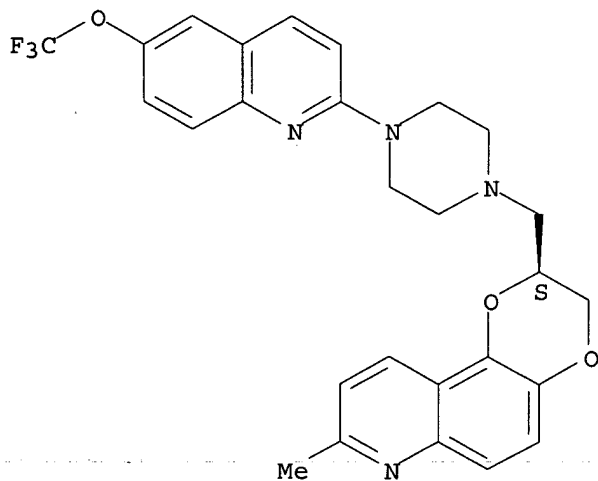
10/659537



RN 676131-33-2 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2,3-dihydro-8-methyl-2-[[4-[6-(trifluoromethoxy)-2-quinolinyl]-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

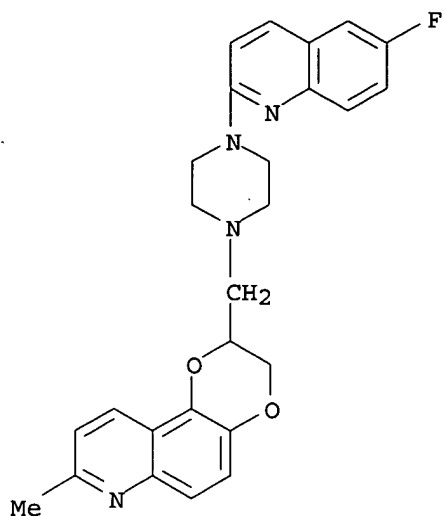
Absolute stereochemistry.



RN 676131-34-3 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(6-fluoro-2-quinolinyl)-1-piperazinyl]methyl]-2,3-dihydro-8-methyl- (9CI) (CA INDEX NAME)

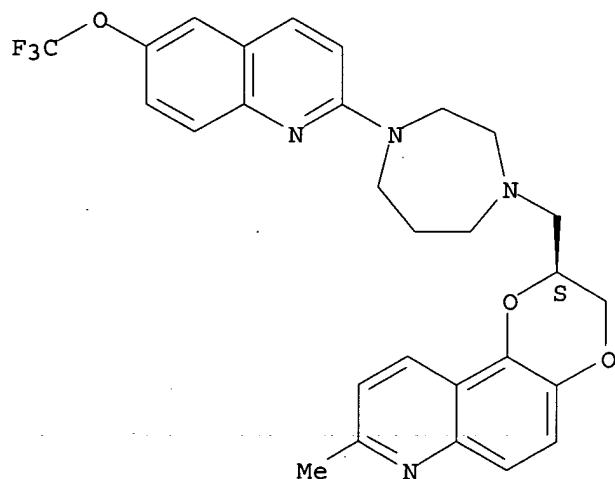
10/659537



RN 676131-35-4 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[hexahydro-4-[6-(trifluoromethoxy)-2-quinolinyl]-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

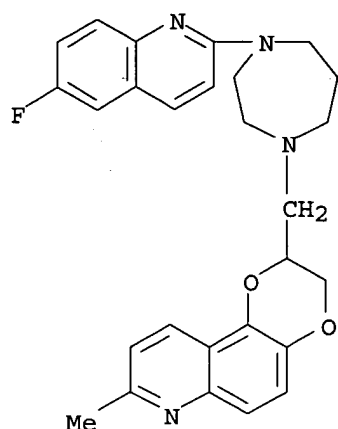
Absolute stereochemistry.



RN 676131-36-5 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(6-fluoro-2-quinolinyl)hexahydro-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl- (9CI) (CA INDEX NAME)

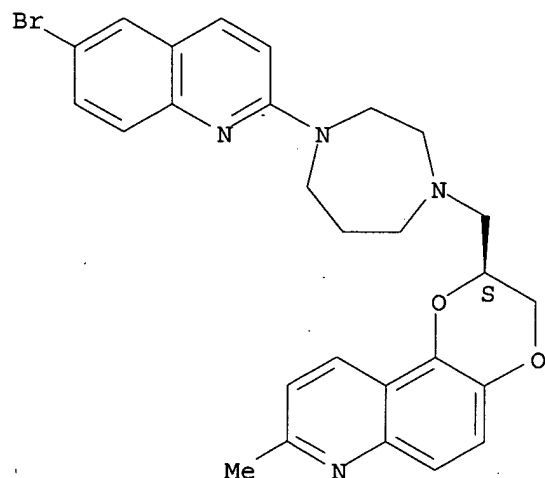
10/659537



RN 676131-37-6 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[4-(6-bromo-2-quinolinyl)hexahydro-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl-, (2S)- (9CI) (CA INDEX NAME)

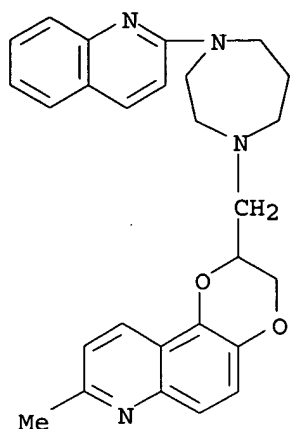
Absolute stereochemistry.



RN 676131-38-7 CAPLUS

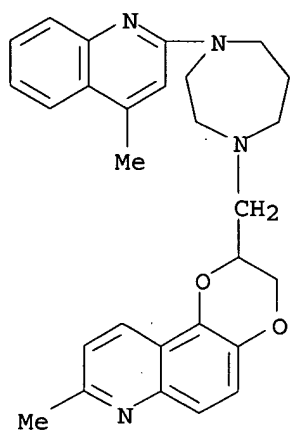
CN 1,4-Dioxino[2,3-f]quinoline, 2-[[hexahydro-4-(2-quinolinyl)-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl-, (9CI) (CA INDEX NAME)

10/659537



RN 676131-39-8 CAPLUS

CN 1,4-Dioxino[2,3-f]quinoline, 2-[[hexahydro-4-(4-methyl-2-quinolinyl)-1H-1,4-diazepin-1-yl]methyl]-2,3-dihydro-8-methyl- (9CI) (CA INDEX NAME)

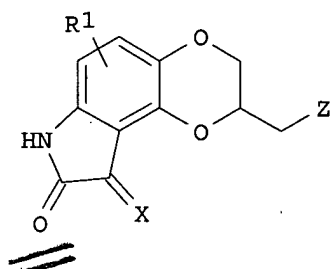


RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/659537

L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:100823 CAPLUS
DN 130:168383
TI Preparation of 2-(azaheterocyclylmethyl)-2,3,8,9-tetrahydro-7H-1,4-dioxino[2,3-e]indol-8-ones as antipsychotics.
IN Stack, Gary Paul
PA American Home Products Corporation, USA
SO U.S., 13 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5869490	A	19990209	US 1997-947565	19971009
PRAI	US 1997-947565		19971009		
OS	MARPAT 130:168383				
GI					



AB Title compds. [I; X = H2, O; R1 = H, OH, halo, CF3, OCF3, alkyl, alkoxy, aralkoxy, alkanoyloxy, amino, alkanamido, alkanesulfonamido; Z = (substituted) piperazinyl, (substituted) (benzo-fused) piperidinyl], were prepared Thus, (R)-(2-tosyloxymethyl)-6-fluoro-2,3,8,9-tetrahydro-7H-1,4-dioxino[2,3-e]indol-8-one and tetrahydroisoquinoline were heated 4 h in Me2SO to give (S)-2-(3,4-dihydro-1H-isoquinolin-2-ylmethyl)-6-fluoro-2,3,8,9-tetrahydro-7H-1,4-dioxino[2,3-e]indol-8-amine, isolated as the fumarate. This showed D2 receptor affinity with IC50 = 0.23 nM.

IT 206355-37-5P 206355-52-4P 220456-58-6P
220456-61-1P

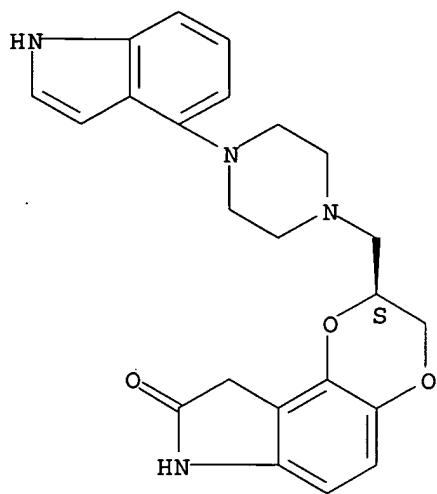
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azaheterocyclylmethyltetrahydrodioxinoindolones as antipsychotics)

RN 206355-37-5 CAPLUS

CN 8H-1,4-Dioxino[2,3-e]indol-8-one, 2,3,7,9-tetrahydro-2-[[4-(1H-indol-4-yl)-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/659537

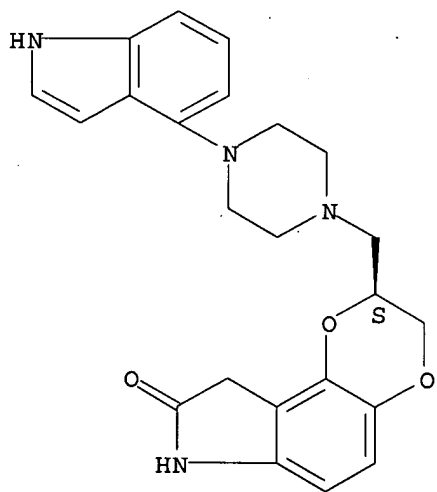


RN 206355-52-4 CAPLUS
CN 8H-1,4-Dioxino[2,3-e]indol-8-one, 2,3,7,9-tetrahydro-2-[[4-(1H-indol-4-yl)-1-piperazinyl]methyl]-, (2S)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 206355-37-5
CMF C23 H24 N4 O3

Absolute stereochemistry.

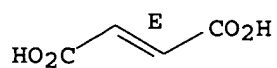


CM 2

CRN 110-17-8
CMF C4 H4 O4

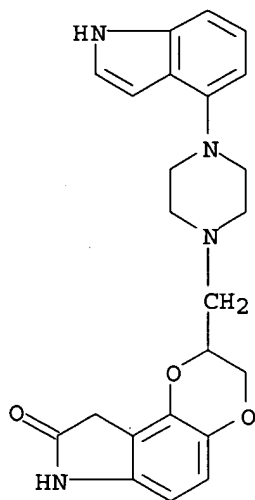
Double bond geometry as shown.

10/659537



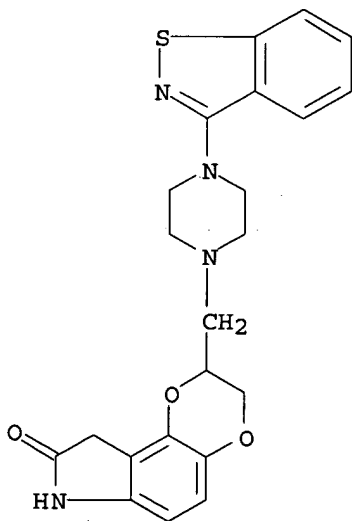
RN 220456-58-6 CAPLUS

CN 8H-1,4-Dioxino[2,3-e]indol-8-one, 2,3,7,9-tetrahydro-2-[[4-(1H-indol-4-yl)-1-piperazinyl]methyl]- (9CI) (CA INDEX NAME)



RN 220456-61-1 CAPLUS

CN 8H-1,4-Dioxino[2,3-e]indol-8-one, 2-[[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]methyl]-2,3,7,9-tetrahydro- (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1998:251174 CAPLUS
 DN 128:308493
 TI Preparation of azaheterocyclylmethyl derivatives of 2,3,8,9-tetrahydro-7h-1,4-dioxino[2,3-e]indol-8-one for the treatment of brain dopamine dysregulation
 IN Stack, Gary Paul
 PA American Home Products Corporation, USA
 SO PCT Int. Appl., 40 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9816530	A1	19980423	WO 1997-US18275	19971010
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2268195	AA	19980423	CA 1997-2268195	19971010
	AU 9748138	A1	19980511	AU 1997-48138	19971010
	EP 932609	A1	19990804	EP 1997-910866	19971010
	EP 932609	B1	20030514		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	JP 2001502327	T2	20010220	JP 1998-518447	19971010
	AT 240335	E	20030515	AT 1997-910866	19971010
	PT 932609	T	20030930	PT 1997-910866	19971010
	ES 2196312	T3	20031216	ES 1997-910866	19971010
PRAI	US 1996-732807	A	19961015		
	WO 1997-US18275	W	19971010		
OS	MARPAT 128:308493				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; X = H₂, O; R₁ = H, OH, halo, etc.; Z = II, III, IV (wherein R₂ = H, C₁-6 alkyl, C₃-8 cycloalkyl, etc.; R₃ = H and R₄ = H, (un)substituted 1-benzimidazolyl-2-one, indolyl, etc.; R₃R₄ taken together with the carbon atom to which they are attached form V or VI; R₅ = H and R₆ = (un)substituted Ph, naphthyl, thienyl, etc.; R₅R₆ taken together with the carbon atoms to which they are attached complete a benzene ring optionally substituted with R₁)] and their salts, useful for the treatment of brain dopamine dysregulation, especially schizophrenia or a schizoaffective disorder, were prepared. Thus, reaction of (R)-2-(toluene-4-sulfonyloxymethyl)-2,3,8,9-tetrahydro-7H-1,4-dioxino[2,3-e]indol-8-one (preparation described) with tetrahydroisoquinoline in DMSO afforded 82% (S)-I [X = H₂; R₁ = H; Z = 3,4-dihydro-1H-isoquinolin-2-yl] which showed IC₅₀ of 0.35 nM against the dopamine D₂ receptor binding.

IT 206355-37-5P 206355-46-6P 206355-52-4P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

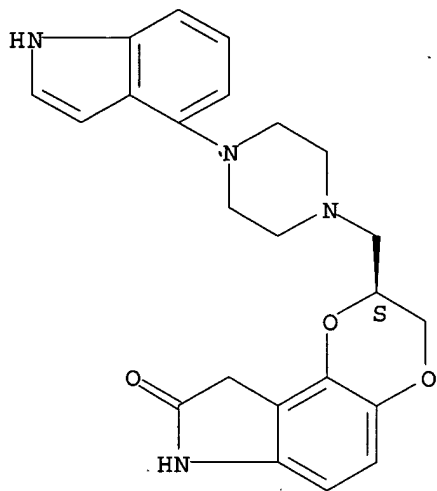
10/659537

BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azaheterocyclomethyl derivs. of 2,3,8,9-tetrahydro-7h-1,4-dioxino[2,3-e]indol-8-one for the treatment of brain dopamine dysregulation)

RN 206355-37-5 CAPLUS

CN 8H-1,4-Dioxino[2,3-e]indol-8-one, 2,3,7,9-tetrahydro-2-[[4-(1H-indol-4-yl)-1-piperazinyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

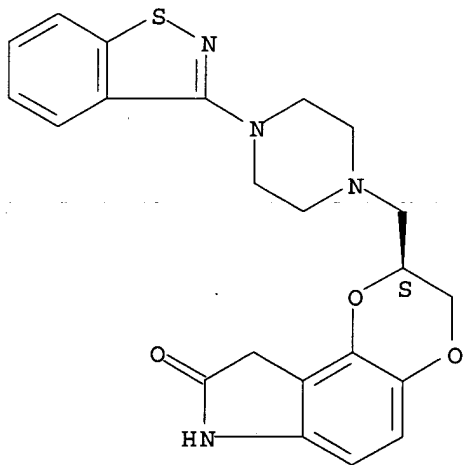
Absolute stereochemistry.



RN 206355-46-6 CAPLUS

CN 8H-1,4-Dioxino[2,3-e]indol-8-one, 2-[[4-(1,2-benzisothiazol-3-yl)-1-piperazinyl]methyl]-2,3,7,9-tetrahydro-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 206355-52-4 CAPLUS

CN 8H-1,4-Dioxino[2,3-e]indol-8-one, 2,3,7,9-tetrahydro-2-[[4-(1H-indol-4-yl)-1-piperazinyl]methyl]-, (2S)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

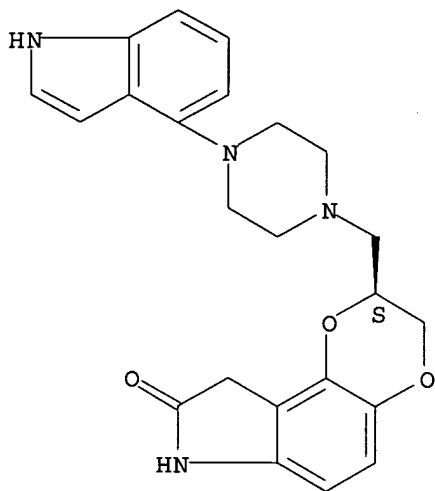
10/659537

CM 1

CRN 206355-37-5

CMF C23 H24 N4 O3

Absolute stereochemistry.

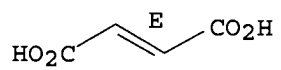


CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



RE.CNT 4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/659537

=> file caold

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L3 54 S L1 SSS FULL

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L4 4 S L3

FILE 'CAOLD' ENTERED AT 16:33:25 ON 07 FEB 2005

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L5 0 L3

=> log h

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CA SUBSCRIBER PRICE	0.00	-2.92

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